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Heat, water, and chemical transport in soils

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Heat, water, and chemical transport in soils

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ABSTRACT

Transport processes of heat, water, and chemicals in soils are very important for managing the root zone for maximum crop production and controlling soil and water quality for minimum degradation and pollution. New and simple analytical or approximate solutions to the corresponding transport problems are presented in this research. Analytical or approximate solutions are further manipulated to estimate the corresponding transport properties. An analytical solution to coupled conduction and convection heat transfer problem under field conditions is obtained by Fourier transformation. The analytical solution can predict field observations of infiltration and temperature well. Three new methods for estimating transport properties in soils are developed in this study. They are: soil water diffusivity determination by general similarity, soil hydraulic property estimation by integral method, and solute transport parameter estimation by boundary layer theory. The general similarity method for water diffusivity determination only requires measuring advance of wetting front with time. The general similarity diffusivities for five soils compare well to those determined by Boltzmann transformation. The integral method estimates soil water characteristic curve and unsaturated hydraulic conductivity simultaneously. The estimated hydraulic properties for six soils ranging from sandy loam to clay loam by the integral method are in good agreement with independently determined values. A boundary layer method for estimating dispersion coefficient and retardation factor is developed. The boundary layer method is applicable both to soil columns and field soils. All of the methods developed in this dissertation present simplifications in application and they are less time consuming than current methods.

CHAPTER 1. GENERAL INTRODUCTION

Introduction

The importance of heat, water, and chemical transport in soils has been long been understood. Theoretical and experimental studies on the transport of heat, water, and chemicals in soils have been further motivated by concerns about the quality of soil and water resources on the earth, as well as by attempts to optimally manage the root zone for maximum crop production and to control soil degradation and groundwater pollution to the limit of soil sustainability and "filtering" capacity.

Much effort has been made to develop a variety of models for describing and predicting the transport processes in soils. The most popular ones are the classical Richards equation for water flow, the Fourier-based conduction-convection equation for heat transfer, and the Fickian--based convection-dispersion equation for solute transport in soils. With the development of more and more sophisticated models, increasing effort has to be made to estimate transport properties of soils in order to model and understand transport processes properly. There are some cases where analytical solutions to transport problems can be found, and then related transport properties such as hydraulic properties and solute transport parameters are estimated by using corresponding analytical solutions. There have been many methods developed for estimating soil transport properties based on the corresponding analytical solutions. However most of them have constraints for application. For example, accuracy, time-consuming, limited range of measurement, and expensive and specialized equipment often restrict practical use of a specific method. This encourages soil physicists to keep looking for new methods that will overcome the above limitations by finding simpler solutions to the corresponding governing equations.

With the preceding sentiment as motivation, the topic of this dissertation was chosen. The research concentrates on finding new and simple analytical solutions to transport processes of heat, water, and chemicals in soils. Much attention is paid to estimate soil transport properties by using new and simple solutions to the transport problems. Thus some innovative methods for estimating soil transport properties are produced in this study, such as soil water diffusivity determination by general similarity theory, soil hydraulic property estimation by integral method, and boundary layer method for estimating solute transport parameters. All new methods are based on corresponding new, simple or more general solutions to corresponding transport problems.

Water is the most important carrier of heat and solutes into soils. More research on unsaturated water flow has been done in this dissertation than on heat transfer and solute transport. However, coupled heat and water transport and solute transport are also involved in this dissertation. Brief introductions to the corresponding topic are provided in order of chapters.

Chapter 2 of this dissertation solves coupled heat and water transport problem for field conditions analytically by using Fourier transformation technique. The analytical solution predicts temperature changes both with time and position well under field conditions. This problem usually needs to be solved by moving boundary theory that involves intensive numerical calculations and only gives implicit solution to the problem.

Chapters 3 and 4 solve horizontal water redistribution problem analytically by using general similarity theory. The general similarity solution can be used to determine soil water diffusivity by only observing the advance of wetting front with time. The general similarity method for water diffusivity improves the traditional Bruce-Klute method by removing the limitation of zero-diffusivity at initial water content no matter how high the initial water content. It is shown that Boltzmann transformation of Bruce-Klute method is only a specific case of the general similarity theory.

Chapters 5 and 6 provide an approximate analytical solution to horizontal water infiltration problem by using integral method. The solution is manipulated to estimate soil hydraulic properties. The integral method for estimating hydraulic properties of soils only needs observation data of sorptivity, length of wetted zone, and saturated hydraulic conductivity to predict soil characteristic curve and unsaturated hydraulic conductivity of a soil that is described by van Genuchten (1980) hydraulic model. This method provides a new and simple means to determine soil hydraulic properties.

Chapter 6 shows an approximate solution to the convection-dispersion equation of solute transport is obtained by using boundary layer theory. The solution is used to determine dispersion coefficient and retardation factor by observing the advance of solute front with time. The observation of solute front can be done by using a tracer solution with a dye. The boundary layer method is applicable both to laboratory and field conditions.

Dissertation Organization

This study is presented in eight chapters. Chapter 1 is general introduction. Chapter 8 is general conclusions. The rest are prepared according to general manuscript requirements for publication in a referred scientific journal. Chapter 2, "Analytical solution for one-dimensional heat conduction-convection equation," was submitted for publication in Soil Science Society of America Journal. Chapter 3, "Soil water diffusivity determination by general similarity theory," was submitted for publication in Soil Science. Chapter 4, "Exact solution for horizontal redistribution by general similarity," will be submitted for publication in either Soil Science Society of America Journal or Soil Science, as will chapters 5, 6, and 7, "Simple water infiltration method for estimating soil hydraulic properties: I. Theoretical analysis," "Simple water infiltration method for estimating soil hydraulic properties: II. Experimental," and "Estimation of solute transport parameters by boundary layer theory," respectively.

CHAPTER 2. ANALYTICAL SOLUTION FOR ONE-DIMENSIONAL HEAT CONDUCTION-CONVECTION EQUATION

A paper submitted to Soil Science Society of America Journal

Mingan Shao, Robert Horton, Dan B. Jaynes

Abstract

Coupled conduction and convection heat transfer occurs in soil when a significant amount of water is moving continuously through soil. Prime examples are rainfall and irrigation. In this paper, an analytical solution for the heat conduction-convection equation is presented. The solution for the upper boundary of first type is basically obtained by Fourier transformation. Results from the analytical solution are compared to observations from a field infiltration experiment with natural temperature variations. The predicted temperature values are very similar to the observed values. Temperature changes with time for different soil depths are predicted from conduction-convection theory and from conduction theory alone. During infiltration, convective heat transfer provided a large contribution for the temperature changes at all soil depths monitored. The theory also predicts temperature effects on surface infiltration quite accurately.

Introduction

In recent decades, efforts have been made to understand the effects of temperature on soil physical and chemical properties. Recent efforts have focused on the modeling of water and heat transfer in soils, together with studying temperature effects on the physical and chemical properties of soils (Nassar and Horton, 1992a; 1992b). Soil hydraulic properties are temperature dependent in part because of the temperature effect on water viscosity. While the effect of temperature on hydraulic properties of a soil has been studied under laboratory conditions (Constantz, 1982), little information on the same topic can be found in field conditions because either the effect may be too small to be worthy of considering (Jaynes, 1990) or the conditions are too complicated to be handled. However, some observations of the temperature effects on infiltration have been made (Musgrave, 1955; Bouwer et al., 1974). Increases in seepage or infiltration rate were observed in response to temperature increases (e.g., Constantz, et al, 1994). Additional mathematical and physical studies may lead to the development of methods for estimating seepage rates based upon soil temperature changes.

Water and heat transfer in soils can be modeled either numerically or analytically. Most research on the modeling of water and heat movement in soils has been made by numerical techniques (Jaynes, 1990; Horton and Chung, 1991; Nassar and

Horton, 1992a; 1992b). Few analytical solutions are available for isothermal water flow in soil (Knight and Philip, 1974; Parlange and Fleming, 1984; Sander et al, 1988; 1991; Barry and Sposito, 1989; Barry and Sander, 1991). Even fewer are available for coupled heat and water transport (Bredehoeft and Papadopulos, 1965; Milly, 1984). Nevertheless it is possible to analytically solve the simultaneous transfer problem of water and heat in soils under certain conditions. New analytical solutions will improve our understanding of coupled heat and water flow problems because the analytical solutions themselves contain more explicit information of process descriptions, model parameters, and initial and boundary conditions than do numerical methods. Analytical solutions will also provide standards for comparing with the numerical solutions. The objective of this paper is to derive an analytical solution to water and heat transfer during infiltration under field conditions. The analytical solution will be compared with field-measured data.

Model

The partial differential equation for one-dimensional simultaneous nonsteady heat and water transfer through isotropic, homogeneous porous medium is (Bredehoeft and Papadopulos, 1965)

$$\frac{c_s\rho_s}{\kappa}\frac{\partial T}{\partial t}=\frac{\partial^2 T}{\partial x^2}-\frac{c_l\rho_l}{\kappa}\frac{\partial (qT)}{\partial x} \tag{1}$$

where T is temperature at any point and at any time (°C), t is time (s), x is the depth (m; positive downwards), κ is soil thermal conductivity (W m^{-1} $°C^{-1}$), c_l and c_s , and ρ_l and ρ_s are specific heats of the liquid and solid (J kg^{-1} $°C^{-1}$), and the liquid and bulk densities (kg m^{-3}), respectively, and q is the liquid infiltration rate or volume flux density (m^3 s^{-1} m^{-2}). The infiltration rate is a function of time. Therefore, for 1-D infiltration into soils, the equation can be reduced to

$$\frac{\partial T}{\partial t}=\frac{\kappa}{c_s\rho_s}\frac{\partial^2 T}{\partial x^2}-q(t)\frac{c_l\rho_l}{c_s\rho_s}\frac{\partial T}{\partial x} \tag{2}$$

If we let $D=\kappa/(c_s\rho_s)$ and $r=c_l\rho_l/(c_s\rho_s)$, then (2) is reduced to

$$\frac{\partial T}{\partial t}=D\frac{\partial^2 T}{\partial x^2}-rq(t)\frac{\partial T}{\partial x} \tag{3}$$

where D is the thermal diffusivity (m^2 s^{-1}).

The initial and typical boundary conditions for (3) are

$$T(x,0)=f(x) \tag{4}$$

$$T(\infty, t) = T_1 \tag{5}$$

$$T(0, t) = T_0 + A\sin(wt+\phi) \tag{6}$$

Where in (5) and (6), T_0 is the average temperature (°C) of the soil surface; A (°C) is the amplitude of surface temperature oscillations of angular frequency w (rad s^{-1}); The term T_1 is defined as a constant temperature at infinite depth, but is usually approximated by the temperature at a relatively large depth; and f(x) (°C) is the initial temperature distribution in the soil profile. Also in (6), the symbol ϕ is for an initial phase angle (radian).

For the case of ponded surface infiltration (Jaynes, 1990), the water flux density, q(t) of (3) may also be expressed by a periodic function of time. We demonstrate this as follows. First we express q(t) as a function of h, the pressure head of soil water.

$$q(t) = -\frac{\eta_r}{\eta_T} K_r(h) \left(\frac{\partial h}{\partial x} - 1\right) \tag{7}$$

where η_r and η_T are the liquid viscosities for a reference temperature and for the current temperature (kg m^{-1} s^{-1}), h is the pressure head of soil water (m), and $K_r(h)$ is the relative hydraulic conductivity (m s^{-1}) determined at the reference temperature.

Second the relative hydraulic conductivity $K_r(h)$ is expressed by Campbell's equation (Campbell, 1974),

$$K_r(h) = K_{sr} \left| \frac{h_a}{h} \right|^n \qquad h < h_a \tag{8}$$

where K_{sr} is the saturated hydraulic conductivity at the reference temperature (m s^{-1}), h_a is the bubbling pressure head (m), and n is a dimensionless constant. For the nearly saturated case of downward seepage described by Jaynes (1990), we may assume that h is constant with a value of $h \geq h_a$ through the profile (unit gradient of soil water potential for the soil profile); then $\partial h/\partial x = 0$, $K_r(h) = K_{sr}$, q(t) is now as

$$q(t) = \frac{\eta_r}{\eta_T} K_{sr} \tag{9}$$

the ratio η_r/η_T in (9) can be approximated by a linear function for the range of temperature variation in field conditions, i.e., we take in (9)

$$\frac{\eta_r}{\eta_T} = V_0 + V_1 T \tag{10}$$

where V_0 (dimensionless) and V_1 ($°C^{-1}$) are constants, and T is the periodic time dependent surface temperature.

For (10) we further take T as

$$T=T_0+A\sin(wt) \tag{11}$$

where T, T_0 and A have dimensions of temperature (°C). A is the same as in (6). Combining (9), (10), and (11), then gives q(t) as

$$q(t)=a_1+b_1\sin(wt) \tag{12}$$

in which $a_1 = K_{sr}\ (V_0 + V_1\ T_0)$ and $b_1 = K_{sr}\ V_1\ A$.

If we let $a = ra_1$ and $b = rb_1$, then from (12), the term, rq(t), in (3) becomes

$$rq(T)=a+b\sin(wt) \tag{13}$$

where from (12) the dimensions of a_1 and b_1 are m s^{-1}.

This completes the model development.

Analytical Solution

The solution to (3) satisfying (4), (5), and (6) may be obtained by transforming (3) into the classical heat equation (Cannon, 1984). The model thus reformulated is a moving boundary problem. Two methods can be employed in the analytical solution. One is Fourier transformation if movement of the boundary is so small that it can be ignored (Powers, 1987). The other is moving boundary approach by use of known mathematical solutions (Cannon, 1984). In this paper, the Fourier transformation method is used because it produces an explicit analytical solution to the problem. We do not use the moving boundary approach because it produces an implicit solution which requires additional intensive numerical integrations. Fourier transforms (Fourier integral), as we use them, are fully detailed in the book of Powers (1987).

Transformation to the Classical Heat Equation

Returning to (3), we can first make a homogeneous boundary condition by means of transformation $T^* = T(x,t)-T_1$. After this transformation and the combination with (13), (3)-(6) become

$$\frac{\partial T^*}{\partial t}=D\frac{\partial^2 T^*}{\partial x^2}-a\frac{\partial T^*}{\partial x}-b\sin(wt)\frac{\partial T^*}{\partial x} \tag{3a}$$

$$T^*(0,t)=(T_0-T_1)+A\sin(wt+\phi) \tag{4a}$$

$$T^*(\infty,t)=0 \tag{5a}$$

$$T^*(x,0)=f(x)-T_1=F(x) \tag{6a}$$

Then, the term, $a\partial T^*/\partial x$, needs to be eliminated. This can be done by the substitution of $U(x, t) = T^* \exp[a^2t/(4D) - ax/(2D)]$. By using this substitution, (3a)-(6a) become, respectively

$$\frac{\partial U}{\partial t} = D\frac{\partial^2 U}{\partial x^2} - [b\sin(wt)]\frac{\partial U}{\partial x} - [\frac{ab}{2D}\sin(wt)]U(x,t) \tag{3b}$$

$$U(0,t) = \exp(\frac{a^2 t}{4D})[(T_0 - T_1) + A\sin(wt+\phi)] \tag{4b}$$

$$U(\infty, t) = 0 \tag{5b}$$

$$U(x,0) = F(x)\exp(\frac{-ax}{2D}) \tag{6b}$$

The next step is to remove the term, $b \sin(wt)\partial U/\partial x$, in (3b). This can be done by introducing a parameter $\lambda_1(t)$ of dimension m which is defined by

$$\lambda_1(t) = \int_0^t b\sin(wt)\,dt = \frac{b}{w}(1-\cos(wt)) \tag{14}$$

Let $z = x - \lambda_1(t)$, then, for function U of (3b) we have $U(x, t) = U(z+\lambda_1(t), t) = V(z, t)$. The differential relationships with respect to time and depth between U and V are given by

$$\frac{\partial U}{\partial t}=\frac{\partial V}{\partial t}-b\sin(wt)\frac{\partial V}{\partial z} \qquad (15)$$

$$\frac{\partial U}{\partial x}=\frac{\partial V}{\partial z} \qquad (16)$$

$$\frac{\partial^2 U}{\partial x^2}=\frac{\partial^2 V}{\partial z^2} \qquad (17)$$

If we combine (15), (16), and (17) with (3b), then we have

$$\frac{\partial V}{\partial t}=D\frac{\partial^2 V}{\partial z^2}-[\frac{ab}{2D}\sin(wt)]V \qquad (18)$$

$$V(-\lambda_1(t),t)=\exp(\frac{a^2 t}{4D})[(T_0-T_1)+A\sin(wt+\phi)] \qquad (19)$$

$$V(\infty,t)=0 \qquad (20)$$

$$V(z,0)=F(z)\exp(\frac{-az}{2D}) \qquad (21)$$

We note that $\lambda_1(t)$ is often small compared to the depth of soil profile concerned. From the field experimental data (Jaynes, 1990), λ_1 is from 0 to 0.04 m (the depth of the profile concerned was 0.6 m).

Analytical Solution of (18) Subject to (19)-(21)

The analytical solution of (18) subject to (19)-(21) may be found by using the Fourier sine transformation, given by

$$V(\lambda,t)=\int_0^\infty V(z,t)\sin(\lambda z)\,dz \tag{22}$$

where λ of dimension m^{-1} is the parameter of the Fourier transformation. By using this transformation, the problem becomes the following initial value problem of an ordinary differential equation

$$\frac{dV(\lambda,t)}{dt}=-[D\lambda^2+\frac{ab}{2D}\sin(wt)]\,V(\lambda,t)+D\lambda\exp(\frac{a^2t}{4D})\,[(T_0-T_1)+A\sin(wt+\phi)] \tag{23}$$

$$V(\lambda,0)=\int_0^\infty F(z)\exp(\frac{-az}{2D})\sin(\lambda z)\,dz \tag{24}$$

Integrating (23) and using the initial condition (24), the explicit analytical solution is expressed as

$$V(\lambda,t)=[I_1+I_3-I_2-I_4+C]\exp[A_3\cos(wt)-D\lambda^2 t] \tag{25}$$

in which

$$I_1 = A_1 \exp(A_2 t) \frac{A_2 \sin(wt+\phi) - w\cos(wt+\phi)}{A_2^2 + w^2} \tag{26}$$

$$I_2 = \frac{I_2^* [(A_2^2+4w^2)\sin(\phi) + A_2^2 \sin(2wt+\phi) - 2A_2 w \cos(2wt+\phi)]}{2A_2(A_2^2+w^2)} \tag{27}$$

$$I_2^* = A_1 A_3 \exp(A_2 t) \tag{28}$$

$$I_3 = (A_4/A_2)\exp(A_2 t) \tag{29}$$

$$I_4 = \frac{A_3 A_4 \exp(A_2 t)\,[A_2 \cos(wt) + w\sin(wt)]}{A_2^2 + w^2} \tag{30}$$

in which A_1, A_2, A_3, A_4, and C are constants given by

$$A_1 = D\lambda A \tag{31}$$

$$A_2 = \left(\frac{a^2}{4D} + D\lambda^2\right) \tag{32}$$

$$A_3 = \frac{ab}{2Dw} \tag{33}$$

$$A_4 = D\lambda(T_0 - T_1) \tag{34}$$

$$C = \exp(-A_3)V(\lambda,0) + I_2(0) + I_4(0) - I_1(0) - I_3(0) \tag{35}$$

in which

$$I_1(0) = \frac{A_1[A_2\sin(\phi) - w\cos(\phi)]}{A_2^2 + w^2} \tag{36}$$

$$I_2(0) = \frac{A_1A_3[(A_2^2+2w^2)\sin(\phi) - A_2 w\cos(\phi)]}{A_2(A_2^2+4w^2)} \tag{37}$$

$$I_3(0) = \frac{A_4}{A_2} \tag{38}$$

$$I_4(0) = \frac{A_2A_3A_4}{A_2^2 + w^2} \tag{39}$$

From (25), the solution to V(z,t) is expressed by

$$V(z,t) = \frac{2}{\pi}\int_0^\infty V(\lambda,t)\sin(\lambda z)\,d\lambda \tag{40}$$

The Analytical Solution to the Original Problem

By the substitutions used, we can obtain the solution to the original problem. From V(z,t) of (40), we can obtain the U(x,t) as

$$U(x,t) = \frac{2}{\pi}\int_0^\infty V(\lambda,t)\sin[\lambda(x-\lambda_1(t))]\,d\lambda \tag{41}$$

Then, $T^*(x,t)$ is given by

$$T^*(x,t) = \exp\left(\frac{ax}{2D} - \frac{a^2t}{4D}\right)U(x,t) \tag{42}$$

The solution to the original problem, equation (2), is given by

$$T(x,t) = T_1 + T^*(x,t) \tag{43}$$

where $T^*(x,t)$ is given by (42) and T_1 by (5). Because Eq. (41) is explicit the final solution (Eq. (43)) is explicit rather than implicit. This is one of the advantages of using Fourier transformation rather than using moving boundary theory which can only give an implicit solution for this problem.

Field Experiment

A detailed description of the field experiment can be found in Jaynes (1990). A brief summary is provided here. Ponded infiltration rates were observed near Phoenix, Arizona. The soil was an Avondale clay loam (fine loamy, mixed, hyperthermic Torrifluventic Haplustoll). The leaching basin method was used in the field infiltration experiment. A 6.1 by 6.1 m area was isolated when an 0.4 m tall sheet metal strip was driven 0.2 m into the ground. The center 3.66 by 3.66 m was divided into four sub-basins, 1.83 m on each side, with similar metal borders.

Soil temperatures were measured by copper-constantan thermocouples. Temperature measurements were observed hourly at depths of 0, 0.05, 0.1, 0.15, 0.2, 0.3, 0.4, 0.5, and 0.6 m. Infiltration rates were measured by flow meters and corrected for changes in measured ponding depth. All of the measurements were continued over a period of 120 h.

Results and Discussion

1. Initial Profile Temperature Distribution

The observed initial soil temperature versus depth can be approximated by the following exponential function,

$$f(x) = T_1 + Be^{-kx} \tag{44}$$

where T_1 (18.02 °C) is the constant temperature when x approaches infinity, B (12.3 °C) and k (19.07 m^{-1}) are coefficients. The result of the best fit for the initial temperature distribution is shown in Fig. 1. From Fig. 1, we can see that the initial temperature may be approximated by the exponential function. With this initial temperature, the needed $V(\lambda, 0)$ of (24) can be expressed as

$$V(\lambda,0) = \frac{B\lambda}{\lambda^2 + (k + \frac{a}{2D})^2} \tag{45}$$

2. Required Parameters

The parameters required in the analytical solution were obtained either from the experiment (Jaynes, 1990) or from calculations. The heat capacity and thermal conductivity of the soil were calculated (Campbell, 1985). Their values are

2090 J kg^{-1} K^{-1} and 1.434 W m^{-1} K^{-1}, respectively. The T_0 (21.5 °C) was calculated using the measured surface temperature. The K_{sr} (at 21.5 ^{0}C) was found to be 0.022 m h^{-1}. The C_1 and ρ_1 are assumed to be 4180 J kg^{-1} K^{-1} and 1000 kg m^{-3}, respectively. The ρ_s was 1.50 Mg m^{-3} by measurement. Daily amplitude of the surface temperature was obtained by fitting a sine function to the observed temperature, the amplitude ranged from 5.85 to 7.25 °C. The w (angular frequency) was assumed to be $2\pi/24$ (rad h^{-1}). The V_0 (0.46, dimensionless) and V_1 (0.02, K^{-1}) were obtained by a linear regression. The viscosity data were taken from Weast (1986). With these parameters, the analytical solution (43) can be obtained by some proper integrations.

3. The Temperature Changes

Measured and fitted surface temperature are shown in Fig. 2. The surface temperature oscillations can be estimated by a simple sine function with amplitude varying from day to day. In general, higher order harmonics (especially the second and third harmonics) are used to describe the surface temperature. However, for the observed data of surface temperature under these specific field conditions and for simplicity, the fundamental harmonic alone is appropriate. Having amplitude vary from day to day is more important than using higher order harmonics. The comparisons of measured temperature with temperature predicted analytically are shown in Fig. 3. Two objective quantitative measures, R^2 and Root Mean Square Error, RMSE, (Willmott et al., 1985), are used to estimate the accuracy of prediction. At depth of 0.1 m (Fig. 3a), R^2 is 0.84 and RMSE is 1.64 (°C). At depth of 0.2 m (Fig. 3b), R^2 is 0.68 and RMSE is 1.72 (°C). At depth of 0.6 m (Fig. 3c), R^2 is 0.65 and RMSE is 1.19 (°C). Therefore RMSE values are within 2°C of the observations. For most of the time, the analytical solution predicts the temperatures within 2°C of the corresponding field observed temperatures. Reasons for the discrepancies between the observed and simulated temperatures may be (1) the assumption of strictly one-dimensional heat transfer and (2) parameter estimations. In reality, heat transfer under the field conditions may be three dimensional. That means lateral heat transfer may occur. Water moving laterally carries heat laterally which results in decreased vertical heat transfer. This may explain why the analytical solution tends to overestimate soil temperatures for all depths. Actual measurement of the parameters in the coupled heat and water transfer should increase the accuracy of temperature prediction of the analytical solution. However this does not affect the analytical approach for understanding the problem itself.

The analytical solution is sensitive to the saturated hydraulic conductivity of the soil. The K_{sr} affects the amplitude of the soil temperature at different depths. This is because percolating water carries heat down the soil profile, particularly important for the deeper depths. This can be shown by comparing the temperature profiles for conduction-convection (percolating water) versus conduction (no water flow) alone. The results of the comparisons are given in Fig. 4 (a, b, and c). The temperature difference between the two mechanisms persists with depth. The convection affects not only the oscillation (amplitude) but also the mean temperature at the deeper depths.

4. Oscillating Surface Infiltration

The surface infiltration rates both measured and predicted are shown in Fig. 5. The flux changed with time somewhat like a sine function. The reason is because surface temperature oscillates with time causing the water viscosity to oscillate with time. As viscosity fluctuates the saturated hydraulic conductivity fluctuates also. Specifically, in the daytime, temperature of water on soil surface increases, then water viscosity decreases, therefore saturated hydraulic conductivity increases and so does infiltration rate. The similar argument can be applied to the night time.

Conclusions

The analytical solution for coupled heat and water transfer under typical field initial and boundary conditions can be obtained by using some variable substitutions and Fourier transformation. The analytical procedure for the solution of heat conduction-convection equation is straight forward and may be useful in checking coupled water and heat numerical procedures. The analytical solution improves our understanding of coupled heat and water transfer problem. One example is the analysis of the relative importance between conductive heat transfer and convective heat transfer. Furthermore the analytical solution itself may provide useful water and heat flux predictions for field conditions when significant water and heat transfer is occurring. For instance, we can use temperature profiles as an indicator for percolation rates of a streambed or seepage rates for a canal. Other appropriate field conditions for application are rainfall infiltration and flood irrigation.

References

Barry, D.A., and G. Sposito. 1989. Analytical solution of a convection-dispersion model with time-dependent transport coefficients. Water Resour. Res. 25: 2407-2416.

Barry, D.A., and G.C. Sander. 1991. Exact solutions for water infiltration with arbitrary surface flux or nonlinear solute adsorption. Water Resour. Res. 27: 2667-2680.

Bouwer, H., R.C. Rice, and E.D. Escarcega. 1974. High-rate land treatment. I: Infiltration and hydraulic aspects of the Flushing Meadows project. J. Water Pollut., 46: 834-843.

Bredehoeft, J.D., and I.S. Papadopulos. 1965. Rates of vertical groundwater movement estimated from the earth's thermal profile. Water Resour. Res. 1: 325-328.

Campbell, G.S. 1974. A simple method for determining unsaturated conductivity from moisture retention data. Soil Sci. 117: 311-314.

Campbell, G.S. 1985. Soil Physics with Basic. pp 31-34. ELSEVIER, Amsterdam.

Cannon, J. R. 1984. The One-Dimensional Heat Equation. Addison-Wesley, Reading, Mass.

Constantz, J. 1982. Temperature dependence of unsaturated hydraulic conductivity of two soils. Soil Sci. Soc. Am. J. 46: 466-470.

Constantz, J., C. L. Thomas, and G. Zellweger. 1994. Influence of diurnal variations in stream temperature on streamflow loss and groundwater recharge. Water Resour. Res. 30: 3253-3264.

Horton, R., and S.O. Chung. 1991. Soil heat flow, *In* Modeling Plant and Soil Systems, Ritchie, J.T. and Hanks, R.J., eds., Agron. Monogr. No. 31, American Society of Agronomy, Madison, WI, 397-438.

Jaynes, D.B. 1990. Temperature variation effect on field-measured infiltration. Soil Sci. Soc. Am. J. 54: 305-312.

Knight, J.H., and J.R. Philip. 1974. Exact solutions in nonlinear diffusion, J. Eng. Math. 8: 219-227.

Milly, P.C.D. 1984. A linear analysis of thermal effects on evaporation from soil. Water Resour. Res. 20: 1075-1085.

Musgrave, G.W. 1955. How much of the rain enters the soil? WATER. THE YEARBOOK OF AGRICULTURE 1955. 151-159.

Nassar, I.N., and R. Horton. 1992a. Simultaneous transfer of heat, water, and solute in porous media: I. Theoretical development. Soil Sci. Soc. Am. J. 56: 1350-1356.

Nassar, I.N., and R. Horton. 1992b. Simultaneous transfer of heat, water, and solute in porous media: II. Experimental and analysis. Soil Sci. Soc. Am. J. 56: 1357-1365.

Parlange, J.-Y., and J.F. Fleming. 1984. First integral of the infiltration equation: 1. Theory. Soil Sci. 137: 391-394.

Powers, D. L. 1987. Boundary Value Problems, Harcourt Brace Jovanovich, Publishers, San Diego.

Sander, G.C., J.-Y. Parlange, V. Kuhnel, W.L. Hogarth, D. Lockington, and J.P.J. O'Kane. 1988. Exact nonlinear solution for constant flux infiltration. J. Hydrol. 97: 341-346.

Sander, G.C., I.F. Cunning, W.L. Hogarth, and J.-Y. Parlange. 1991. Exact solution for nonlinear, nonhysteretic redistribution in vertical soil of finite depth. Water Resour. Res. 27: 1529-1536.

Weast, R.C. (ed. in chief) 1986. CRC Handbook of Chemistry and Physics, CRC Press, Inc., Boca Raton, Florida.

Willmott, C.J., S.G. Ackleson, R.E. Davis, J.J. Feddema, K.M. Klink, D.R. Legates, and C.M. Rowe. 1985. Statistics for the evaluation and comparison od models. J. Geophy. Res. 90: 8995-9005.

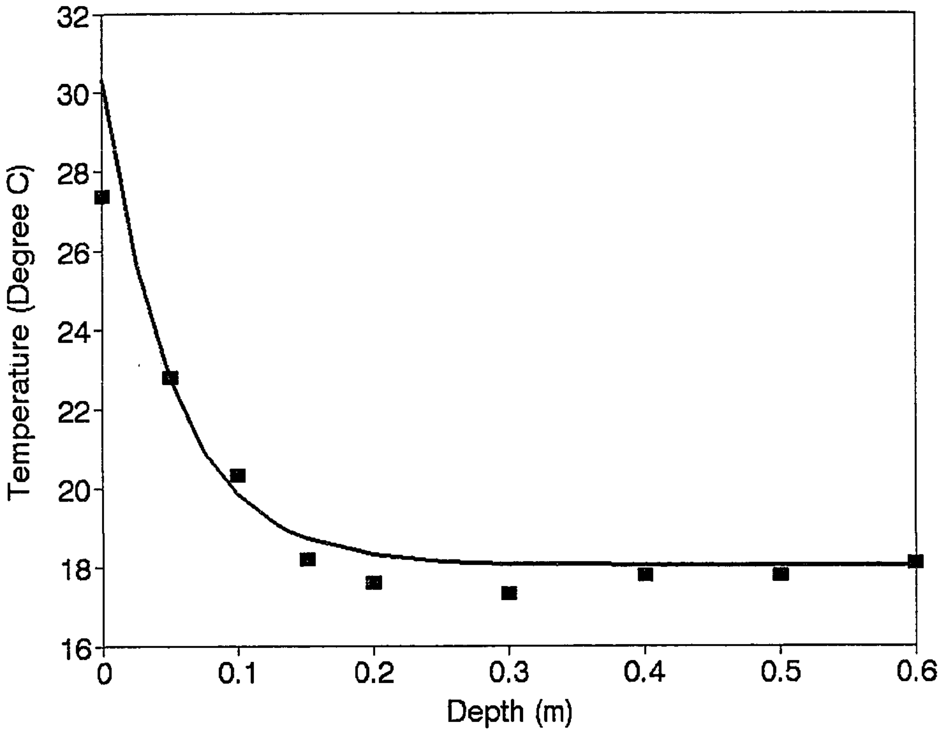

Figure 1. The initial temperature distribution of the soil profile, filled square -- measured and solid curve -- fitted by exponential function.

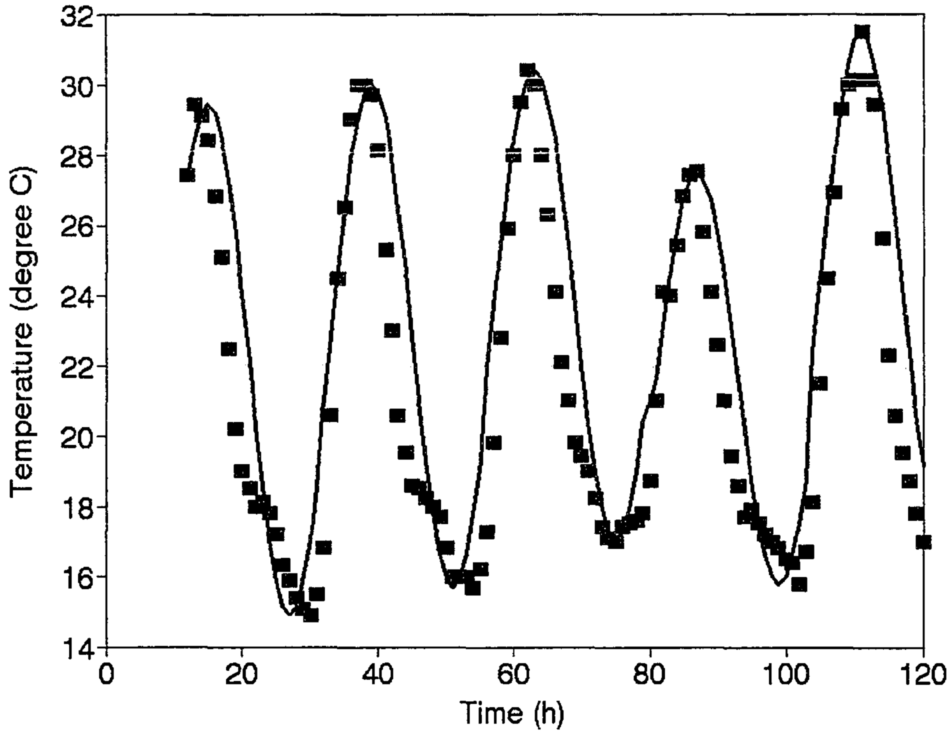

Figure 2. The change of the soil surface temperature with time, filled square -- measured and solid curve -- fitted by sine function.

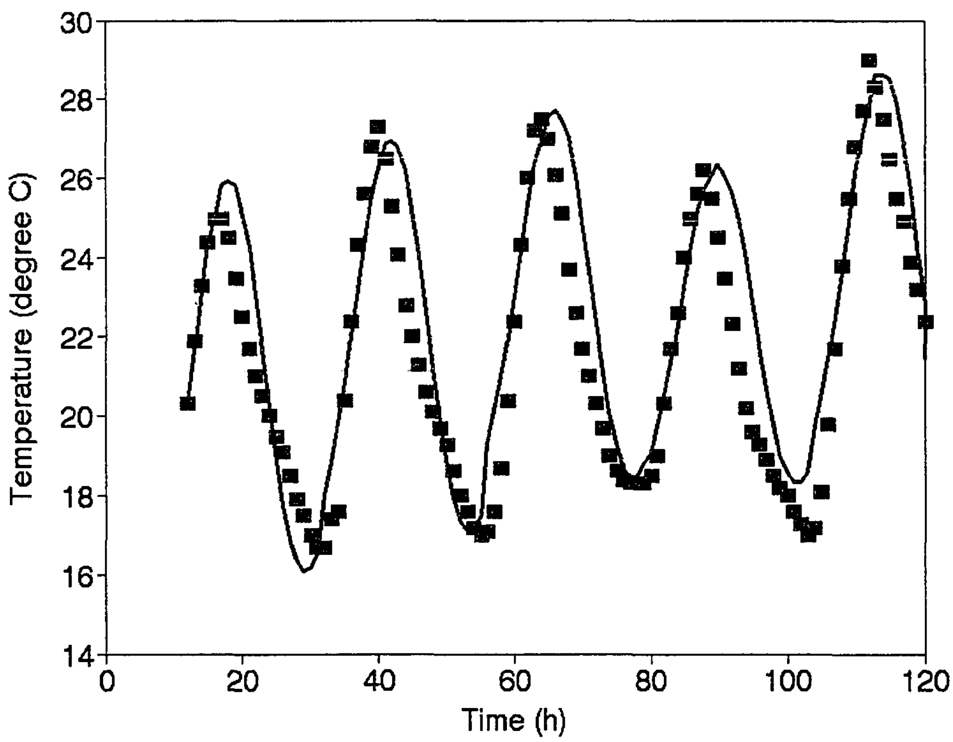

Figure 3a. Comparison of the analytical solution of the soil temperature with the observed temperatures at 0.1 m, filled square--measured and solid curves -- predicted.

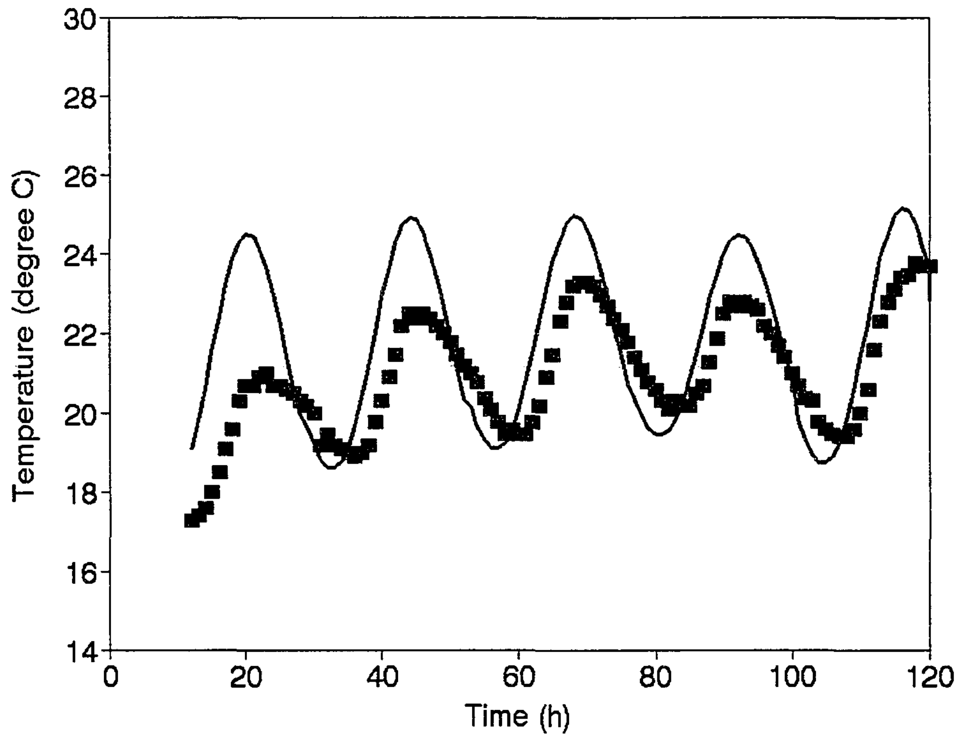

Figure 3b. Comparison of the analytical solution of the soil temperature with the observed temperatures at 0.3 m, filled square--measured and solid curves -- predicted.

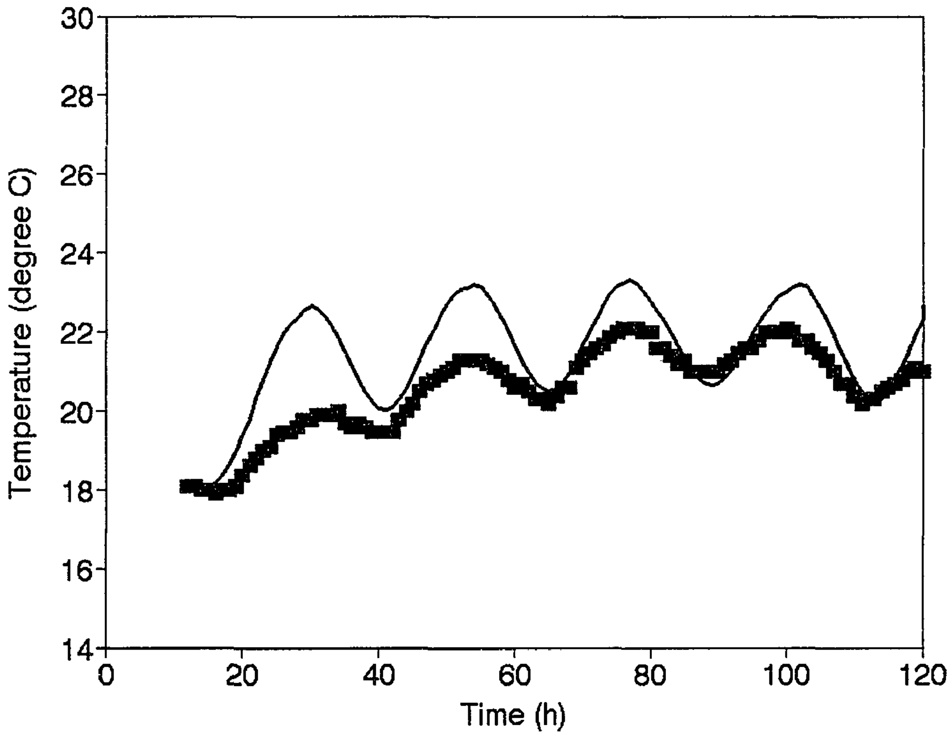

Figure 3c. Comparison of the analytical solution of the soil temperature with the observed temperatures at 0.6 m, filled square--measured and solid curves -- predicted.

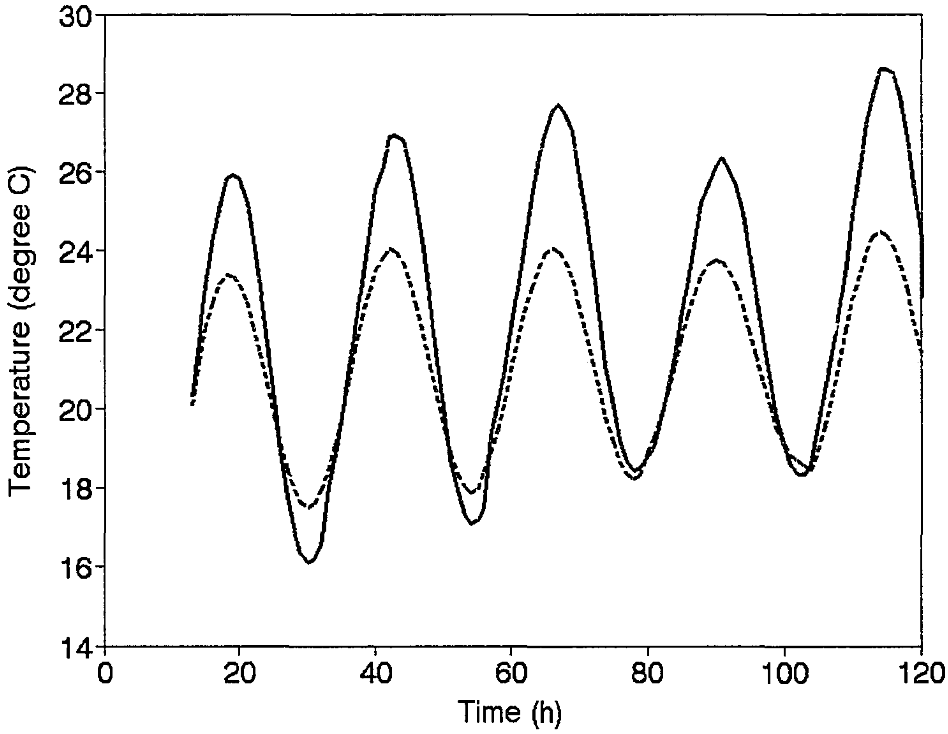

Figure 4a. Comparison of soil temperatures by conduction-convection (solid curves) with those by conduction alone (dashed curves) at 0.1 m.

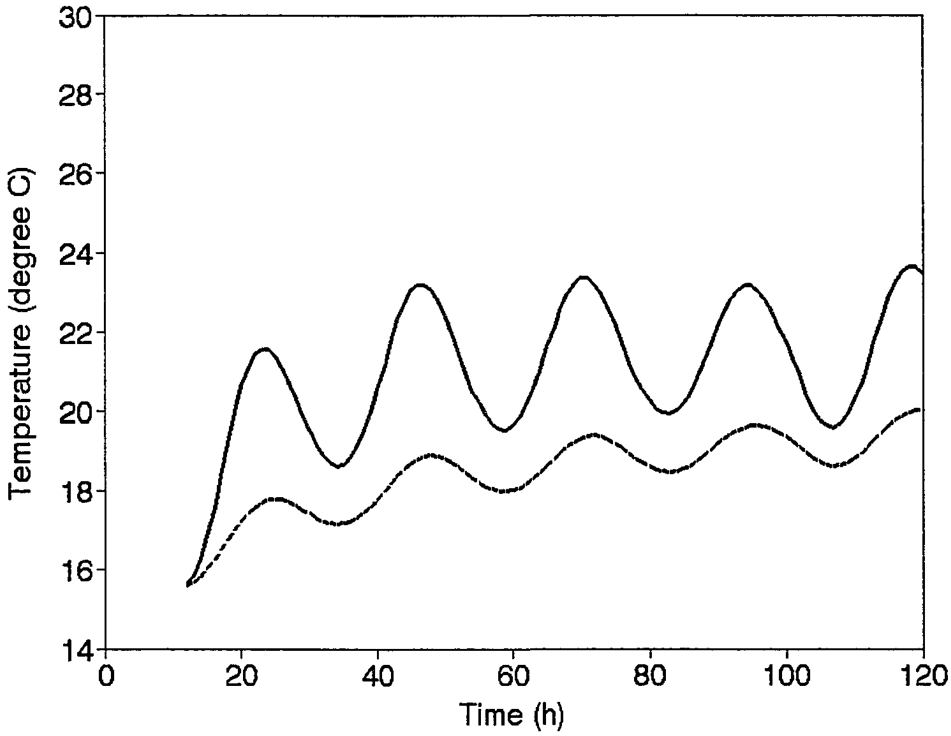

Figure 4b. Comparison of soil temperatures by conduction-convection (solid curves) with those by conduction alone (dashed curves) at 0.3 m.

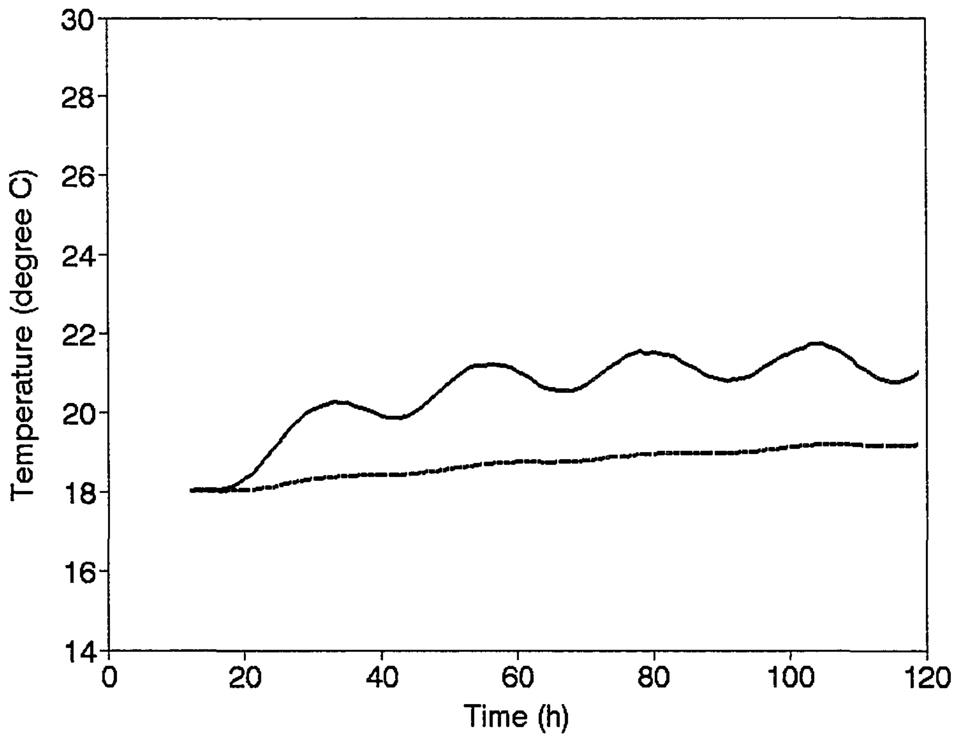

Figure 4c. Comparison of soil temperatures by conduction-convection (solid curves) with those by conduction alone (dashed curves) at 0.6 m.

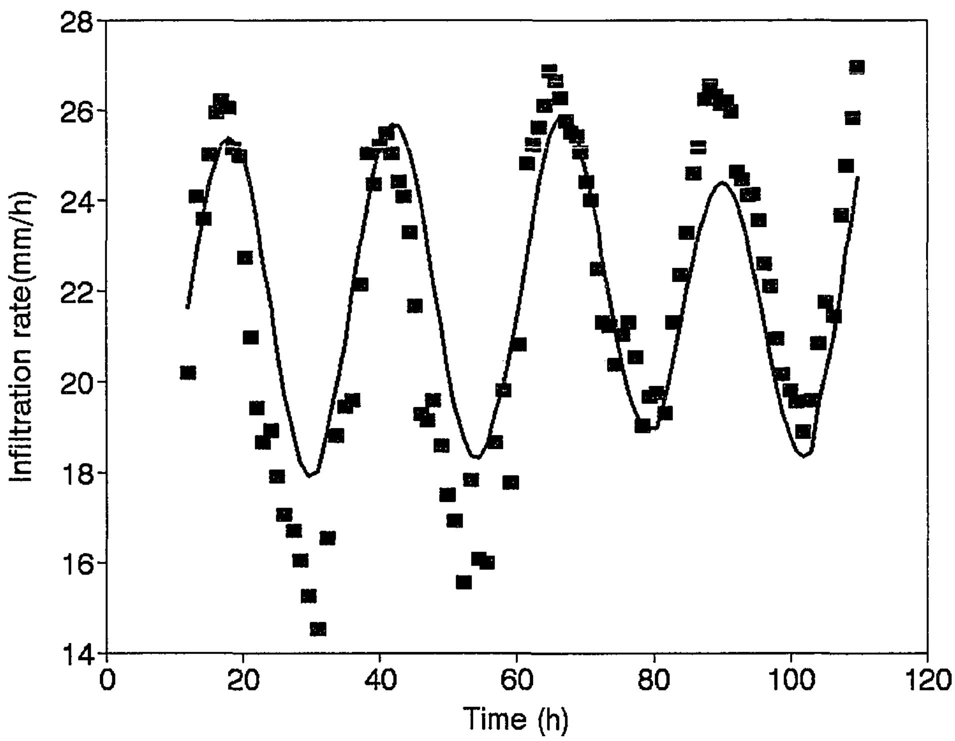

Figure 5. The change of infiltration rate (surface flux) with time, filled square -- measured and solid curve -- predicted.

CHAPTER 3. SOIL WATER DIFFUSIVITY DETERMINATION BY GENERAL SIMILARITY THEORY

A paper submitted to Soil Science

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Abstract

A new and simple method is developed to estimate soil water diffusivity. The method utilizes general similarity theory rather than the Boltzmann transformation to evaluate horizontal water infiltration-redistribution processes. The method uses the Brooks and Corey function of water diffusivity. The method only requires measuring wetting front advance with time. The general similarity diffusivities for five soils were compared with those obtained by Boltzmann transformation and a third method that used a fitting function to approximate the water distribution data in the Boltzmann transformation method. The comparisons showed that soil water diffusivities for the three methods were in good agreement for the intermediate range of water contents. At the low water contents the similarity water diffusivities differed from the other water diffusivities for the five soils. The new method has several advantages over the other methods for determining soil water diffusivity. The new method allows the inlet boundary water content to vary in time and initial water content distribution to vary with distance,

which is more general than constant water content. The new method does not require soil water diffusivity to be zero at the initial water content. This represents an improvement over the earlier methods, which give a zero diffusivity at initial water content no matter how high the initial water content.

Introduction

Soil water infiltration rates and subsequent water redistribution are important concerns for development of soil management practices to minimize potential groundwater contamination from land applied chemicals. Numerical solutions of the flow and transport problems in the vadose zone are the most important approaches to predict quantitatively the dynamic behavior of the system. The unsaturated flow and transport modeling usually requires accurate and complete information about the unsaturated hydraulic properties for the model to function properly. There are three basic hydraulic parameters: hydraulic conductivity (K), water diffusivity (D), and specific water capacity (C). Among the three parameters, only two of them are independent because of the relationship K= CD.

In recent years, increasing efforts have been made toward determining water diffusivities of unsaturated soils. Usually, horizontal infiltration experiments have been used to relate the soil water diffusivity to the volumetric water content by the method of Bruce and Klute (1956). The method is based on the Boltzmann transformation and constant initial condition, zero flux upper boundary, and constant water content lower boundary conditions. The water content distribution along the column needs to be measured in order to estimate the water diffusivity. The most common way for finding D was shown by Kirkham and Powers (1972, p. 256). There are difficulties in determining the slope of the water distribution curve. Cassel et al. (1968) presented a method for estimating soil water diffusivity values based on time-dependent soil water content distribution in the horizontal redistribution process. Their method needs water content distribution with time to be measured and also involves both relatively intensive calculation and long time running of the experiments. Clothier et al. (1983) presented a fitting function chosen from those presented by Philip (1960) to approximate the water distribution curve in the Bruce-Klute method (1956). This makes a simple analytical expression of the water diffusivity possible by avoiding finding the slopes of the soil water distribution curve. However, the method of Clothier et al.(1983) needs precise measurements for parameter estimation of their analytical expression of water diffusivity; for example, a small error in determining the water content of the inlet boundary with their formula may produce a negative p value (Eq.(15) in their paper), which makes no physical sense. McBride and Horton (1985), based on the Bruce-Klute method (1956), used various aspects of this approach to develop a method of determining the water diffusivity from horizontal infiltration experiments. Particularly, they introduced an empirical function, fitted by least squares regression to water distribution data. Their approach provides another way to determine the water diffusivity. However, the McBride and Horton approach involves intensive calculations. Warrick (1994) gave a detailed review on soil water diffusivity estimation for fixed water content at the inlet boundary. To our knowledge, little information in the literature deals with variable water content of the inlet boundary in the horizontal infiltration experiments for the purpose of diffusivity determination. However, Anderson and Jeppson (1984) developed a nonlinear diffusion model for semiconductors. They found that at high concentration, impurity diffusion in semiconductors tends to be governed by nonlinear diffusion processes. They used a general similarity approach to deal with nonlinear diffusion processes. Their idea may be used in determining the soil water diffusivity; general similarity theory, rather than the Boltzmann transformation, may be used to give an analytical solution of the horizontal infiltration and the redistribution to get an analytical expression of the water diffusivity for variable water-content of the inlet boundary. One factor associated with water redistribution is capillary hysteresis. A complete analysis of water redistribution in soil should take capillary hysteresis effects into account. Currently, only numerical techniques can actually incorporate hysteresis effects into the water flow model. However, analytical solution of nonhysteretic flow may still have certain applications to soil water redistribution. There is some evidence (Watson and Sardana, 1987) that the size of the hysteresis loop decreases for fine-textured soils. Moreover, both theoretical analysis and experimental evidence show that hysteresis has much less effect on hydraulic properties if they are expressed in water content rather than pressure head (Mualem, 1976). The hysteresis phenomenon primarily affects hydraulic properties of soils in the range of capillarity, i.e. in the wet end of hydraulic properties. Therefore nonhysteretic solutions still have applications to water redistribution for certain soil water conditions. Such nonhysteretic solutions should be applicable to certain intermediate and low ranges of soil water content.

This paper presents a method for estimating water diffusivities of unsaturated soils by using a nonhysteretic analytical solution to horizontal redistribution, based on general similarity theory. This new method allows the water content of the inlet boundary to be variable with time and allows the initial water content distribution to be variable with distance. It only needs information on the advance of the wetting front with time to obtain water diffusivities of unsaturated soils. The analytical expression of the water diffusivity will be compared with $D(\theta)$ data for five soils derived from one-dimensional horizontal absorption experiments by the method of Bruce and Klute (1956) and by the method of Clothier et al. (1983).

Theory

For one-dimensional horizontal flow, the flow equation is given by (Klute, 1952)

$$\partial\theta/\partial t = \partial(D(\theta)\partial\theta/\partial x)/\partial x \qquad (1)$$

where $\theta(x,t)$ is the volumetric water content (m^3/m^3), t is the time (s), x is the distance (m), and D is the soil water diffusivity (m^2/s).

The problem to be solved is a two-step problem. First, water infiltrates into the soil, then the water supply is stopped, and the soil water is allowed to redistribute. Our interest is focused on the second step, i.e., the redistribution process. The initial and boundary conditions for the problem of horizontal redistribution are

$$\theta(x, 0) = f(x) \qquad x \le x_0 \qquad (2a)$$

$$\theta(x, 0) = \theta_i \qquad x > x_0 \qquad (2b)$$

$$q(0, t) = - D(\theta)\ \partial\theta(0, t)/\partial x = 0 \qquad (3)$$

$$\theta(x_f, t) = \theta_i \qquad (4)$$

in which x_0 is the initial wetting distance from the inlet end of the soil column to where the water content profile intersects the x axis, $f(x)$ is the water content distribution of the infiltrated water, θ_i is the initial water content in the dry zone, $q(0, t)$ is the flux density at the zero-position boundary (in general, flux density $q=q(x,t)$), and x_f is the position of the wetting front.

Simplifying assumptions are needed to solve the nonlinear flow equation analytically for this particular flow problem. First of all, we adopt the Brooks and Corey water diffusivity (1964), a power function of the water diffusivity, that has been used by others (Parlange et al., 1980; Parlange and Fleming, 1984; Hogarth et al., 1989; Ross and Parlange, 1994a and 1994b), i.e.:

$$D(\theta) = D_0\, \theta^{\gamma} \tag{5}$$

where D_0 and γ are constants.

For the sake of simplicity, let θ_i = constant, and particularly let $\theta_i = 0$ (water redistribution into an oven-dry soil). This assumption was also used in solving the diffusivity equation by Parlange et al. (1980). With these assumptions, the problem can be reduced as follows:

$$\partial\theta/\partial t = \partial(D_0\theta^{\gamma}\, \partial\theta/\partial x)/\partial x \qquad 0 < t\ ,\ 0 < x < \infty \tag{6}$$

$$\theta(x,\ 0) = 0 \qquad x_0 < x < \infty \tag{7}$$

$$\partial\theta(0,\ t)/\partial x = 0 \qquad 0 < t \tag{8}$$

$$\theta(x_f,\ t) = 0 \qquad 0 < t \tag{9}$$

By introducing $\tau = D_0\, t$, then (6) is transformed as

$$\partial\theta/\partial\tau = \partial(\theta^{\gamma}\ \partial\theta/\partial x)/\partial x \tag{10}$$

By using similarity methods, the solution to (10) is written as

$$\theta = \tau^{\alpha}\ \phi(\xi) \tag{11}$$

$$\xi = x/\tau^{\beta} \tag{12}$$

Inserting (11) and (12) into (10), then LHS of (10) is

$$\partial\theta/\partial\tau = \alpha\tau^{\alpha-1}\ \phi(\xi) - \beta\tau^{\alpha-1}\ \xi\ d\phi(\xi)/d\xi \tag{13}$$

The RHS of (10) is

$$\partial\ (\theta^{\gamma}\ \partial\theta/\partial x)/\partial x = \tau^{\alpha\gamma+\alpha-2\beta}\ d(\phi^{\gamma} d\phi(\xi)/d\xi)/d\xi \tag{14}$$

Combining (13) with (14) and dividing both sides by $\tau^{\alpha-1}$ yields

$$\alpha\phi - \beta\xi\ d\phi/d\xi = \tau^{\alpha\gamma-2\beta+1}\ d(\phi^{\gamma}\ d\phi/d\xi)/d\xi \tag{15}$$

In order to remove τ as an explicit variable in (15), the power of τ should be zero, then

$$\alpha = (2\beta - 1)/\gamma \tag{16}$$

and the resulting equation for $\phi(\xi)$ is then

$$\alpha\phi - \beta\xi\ d\phi/d\xi = d(\phi^{\gamma}\ d\phi/d\xi)/d\xi \tag{17}$$

Equation (17) is equation (13) of Hogarth et al. (1989), when the gravity term that is considered in that paper as well, is removed. Hogarth et al. (1989) solved the ordinary differential equation (Eq.(13) in their paper) numerically by a shooting procedure. Particular interest of this paper is to solve equation (17) analytically. Boundary conditions are needed to solve (17). The boundary conditions described by (8) and (9) are transformed as

$$d\phi(0)/d\xi=0 \tag{18}$$

$$\phi(\xi_f)=0 \tag{19}$$

By performing the general similarity transformation, the mixed problem of PDE (equations (6)-(9)) is reduced to a two-point ODE boundary value problem, given by (17)-(19).

By using the initial condition (7) and mass conservation condition, i.e.:

$$\int_0^\infty \theta(x,\tau)dx = \tau^{\alpha+\beta} \int_0^\infty \phi(\xi)\ d\xi \ = H_0 \tag{20}$$

where H_0 is the water applied in the infiltration process (m), of course, H_0 is a constant because the total quantity of water within the redistribution is unchanging during the process of water redistribution. H_0 is also the total quantity of water (H) in the soil column because of zero-initial water content. This statement is also true for non-zero initial condition but the total quantity of water should consist of applied water infiltrated into the column (H_0) and residual water in the soil column (H_r), i.e: $H=H_0+H_r$. Therefore H_0 cannot depend explicitly on τ. To remove any explicit τ dependence, we must have $\alpha = -\beta$, which, together with relation (16), determines α and β to be

$$\alpha = -\beta = -1/(2 + \gamma) \tag{21}$$

With α and β given by (21), (17) with the boundary conditions of (18) and (19) can be integrated explicitly to yield

$$\phi(\xi) = \phi_0 \; (1 - \xi^2/\xi_f^{\,2})^{1/\gamma} \tag{22}$$

In the first integration of (17), (18) is used to give a zero integration constant. In the second integration, (19) is used to determine the integration constant. In (22), the general similarity variable at wetting front, ξ_f, is related to the integration constant, ϕ_0, by

$$\xi_f^{\,2} = 2\phi_0^{\,\gamma} \; (2 + \gamma)/\gamma \tag{23}$$

Furthermore, the integration constant, ϕ_0, is found by inserting (22) into the second integral of (20), i.e.:

$$\phi_0 = (H_0^{\,2} \; \gamma/(2(2 + \gamma) I_\gamma^{\,2}))^{1/(2+\gamma)} \tag{24}$$

where I_γ is a definite integral expressed as

$$I_\gamma = \int_0^1 (1-x^2)^{1/\gamma} \, dx = B(1/2,\; 1+1/\gamma)/2 \tag{25}$$

where $B(1/2,\ 1+1/\gamma)$ is a Beta function, the substitution of $t=x^2$ is used to convert the definite integral to the formal Beta function. The numerical evaluation of the Beta function can be found in Abramowitz and Stegun (1972).

Combining (23) and (24), ξ_f is obtained as

$$\xi_f = (2H_0^{\,\gamma}(2 + \gamma)/(\gamma I_\gamma^{\,\gamma}))^{1/(2+\gamma)} \tag{26}$$

and the wetting front, x_f, is written as

$$x_f(\tau) = (2(2 + \gamma)H_0^\gamma \tau/(\gamma I_\gamma^\gamma))^{1/(2+\gamma)} \tag{27}$$

It is obvious that (27) gives $x_f(0)=0$. That means the given amount of water (H_0) is concentrated at $x_0=0$ with an infinite θ. This is clearly unphysical. We assume that $x_f(0)=x_0$ (a finite distance) over which H_0 is distributed. Then, the solution to the original wetting front, $x_f(t)$, is

$$x_f(t) = x_0 + (2(2 + \gamma) H_0^\gamma D_0 t/(\gamma I_\gamma^\gamma))^{1/(2+\gamma)} \tag{28}$$

Equation (28) is physical now. However experimental data will be used to verify equation (28). It is obvious that equation (28) can be expressed by

$$x_f(t) = x_0 + a t^b \tag{29}$$

The two constants, a and b, in (29) can be obtained experimentally by fitting (29) to the wetting front with time observed in the horizontal infiltration-redistribution experiment.

With a and b, then, γ and D_0 are obtained as follows

$$\gamma = 1/b - 2 \tag{30}$$

$$D_0 = a^{\gamma+2} \gamma I_\gamma^\gamma/(2(2+\gamma)H_0^\gamma) \tag{31}$$

So far, $D(\theta)=D_0\theta^\gamma$ is determined by (30) and (31).

Experiments

Five soils were used to test the approach in this study: a silt loam obtained from land mapped as Flagler series (Coarse-loamy, mixed, mesic Typic Hapludoll, 0.114 sand, 0.700

silt, and 0.186 clay mass fractions), Nicollet loam (Fine-loamy, mixed, mesic Aquic Hapludoll, 0.509 sand, 0.326 silt, and 0.165 clay), Keswick sandy clay loam (Fine, Montmorillontic, mesic Aquic Hapludoll, 0.677 sand, 0.113 silt, and 0.210 clay), Monona silty clay loam (Fine-silty, mixed, mesic Typic Hapludoll, 0.024 sand, 0.695 silt, and 0.281 clay), and Webster clay loam (Fine-loamy, mixed, mesic, Typic Endoaquoll, 0.321 sand, 0.392 silt, and 0.287 clay). The specific surface areas were measured by using EGME technique (Chihacek and Bremner, 1979; Carter et al., 1986). Particle densities were determined by using the pycnometer method (Blake and Hartge, 1986). The inlet boundary water contents of -0.03 m water potential, used in the horizontal infiltration and distribution experiments, are listed in Table 1. These water contents are needed to calculate diffusivity by the method of Clothier et al. (1983).

Table 1. Some physical properties of the five soils

soil	specific surface	particle density	inlet water content
	(10^{-3} m^2/kg)	(Mg/m^3)	(m^3/m^3)
silt loam	41	2.67	0.454
loam	40	2.69	0.460
sandy clay loam	58	2.64	0.447
silty clay loam	79	2.67	0.462
clay loam	141	2.57	0.469

Two types of experiments were carried out to obtain soil water diffusivity data. One was the traditional horizontal-infiltration experiment of the Bruce-Klute method. Air-dried soil was packed into sectioned plexiglas tubes 0.15 m long (15 sections) and 0.038 m in diameter with the controlled bulk density of 1.30 Mg/m^3. A -0.03 m water tension was applied to the inlet boundary of the soil column. This tension was used to reduce water movement along the tube wall. The second was a horizontal experiment of infiltration and redistribution to obtain the two coefficients of the power function of the water diffusivity based on the general similarity theory in this paper. In the second experiment, the oven-dried soil was packed into plexiglas tubes 0.3m long and 0.038m in diameter. The bulk density in the second experiment was the same as that in the Bruce-Klute method. A given amount of water (H_0) was applied to each soil column. For example the amount of water for silt loam soil was 0.003 m . Two methods were used to apply H_0. The first approach was to have H_0 water infiltrate into the soil vertically. After infiltration the column was laid down horizontally while the redistribution of the infiltrated water took place. The second approach was to have H_0 water applied to a separate end section of the soil column and then to connect the end section with the water to a dry soil column. During redistribution, the advance of the wetting front with time was recorded. It was easier to observe $x_f(t)$ for the second approach than for the first way.

Results

1. Parameter Estimation from the Advance of Wetting Front

As mentioned above, the advance of the wetting front with time is measured in the experiment. This advance can be theoretically approximated by Eq.(29). The a and b parameters are related to D_0 and γ in Eq. (5), which describes the water diffusivity by the power function. The a and b parameters are estimated by least squares regression of fitting the observed data of the advance of wetting front with time by a power function. As an example, the analysis of the silt loam is listed in Table 2. D_0 and γ in Table 2 are calculated by using Eqs. (30) and (31). The fitting of the advance of the wetting front with time by a power function with observed data is shown in Fig. 1. Coefficient of determination, R^2, of the fitting is 0.95. Root Mean Square Error, RMSE, (Willmott et al., 1985), is 0.6 mm. Therefore, Eq. (28) describes the wetting front with time well.

Table 2. The parameter values for three samples of silt loam

Column	a (10^{-3}m/s^b)	b	γ	D_0 (10^{-5}m^2/s)
1	6.49	0.191	3.236	9.86
2	6.57	0.195	3.134	10.03
3	6.62	0.194	3.164	10.22
mean	6.56	0.193	3.178	10.04

2. The Water Diffusivity of the Five Soils

The water diffusivities of the general similarity theory for the five soils are obtained by finding the two parameters, γ and D_0, using the observed data of the advance of wetting front with time in the same way as in the above paragraph. The γ and D_0 values estimated by this method are listed in Table 3.

Table 3. Water diffusivity parameters of the five soils

soil	γ (dimensionless)	D_0 (10^{-5} m^2/s)
silt loam	3.18	10.0
loam	3.47	11.2
sandy clay loam	2.85	1.12
silty clay loam	3.34	2.66
clay loam	3.14	1.69

With the parameters in Table 3, the water diffusivity functions of the five soils can be obtained from Eq. (5).

Discussion

The soil water diffusivity of general similarity theory is determined by Eqs.(30) and (31). Because the values of γ and D_0 are dependent on a and b constants in Eq. (29), it may be interesting to look at the sensitivities of the diffusivity to a and b coefficients in Eq.(29). For a given b, i.e., a fixed γ (here b is assumed to be 0.2, then γ is 3), from Eq.(31) it is clear that D_0 will increase 32 times when a is doubled. This is also shown in Fig. 2. Therefore, the a-constant only affects the magnitude of the diffusivity function. However, for a given a-constant (assumed to be 1 cm/min^b), the value of the b-constant affects both the shape and the magnitude of the diffusivity function (Fig. 3). The major effect of the b-constant on the water diffusivity function is the shape of the curve. The smaller the value of b, the steeper the curve. The smaller the value of b, the smaller the value of the diffusivity at lower water content, and the larger the value of the diffusivity at higher water content. Parameter a largely influences the magnitude of the diffusivity, and b largely influences the shape of the diffusivity function.

The water diffusivities by general similarity theory are compared with those obtained by the Bruce-Klute method (1956) and the method of Clothier et al. (1983). The results of the comparisons are shown in Fig. 4. The Bruce-Klute method (1956) provides relatively accurate determination of soil water diffusivity only in intermediate range of water contents (the shoulder of the corresponding water content distribution) because the Bruce-Klute method has difficulty to obtain the slopes at small and large water contents. Therefore particular attention should be given to the water diffusivities at intermediate water contents. The similarity water-diffusivities and water diffusivities by the Bruce-Klute method for all five soils in the intermediate range of water contents (0.15-0.30 of water contents) are in very good agreement. The Clothier et al. method (1983) tends to overestimate water diffusivities for sandy clay loam and underestimates water diffusivities for silt loam at intermediate water contents. At lower water contents, similarity water diffusivities are consistently lower than the other two water diffusivities for all five soils. The differences for all five soils are within one order of magnitude. However the two water diffusivites by the Bruce-Klute method (1956) and the Clothier et al. method (1983) do depend on the initial water content of the soil because both methods give zero water diffusivity at the initial water content. It is not difficult to imagine that there is a jump in water diffusivity near initial water content. The greater the initial water content the bigger the jump. There is uncertainty in water diffusivities by the two methods (Bruce-Klute and Clothier et al. methods) because of the assumption of the zero water diffusivity at initial water content and the inaccurate estimations of the slopes for lower water contents. Therefore the water diffusivity differences for small water contents between the similarity theory method and the other two methods are expected. The water diffusivities from the Bruce-Klute method and the Clothier et al. method are similar for all five soils. These results are expected because both methods have basis on the same Boltzmann transformation theory.

In the redistribution process, the transformation variable is $\xi = x/t^{\beta}$ (here β ranged from 0.18 to 0.21 for the five soils in this study) rather than the Boltzmann variable ($x/t^{0.5}$) used in the Bruce-Klute method (1956). β is not fixed to the value 0.5, but it can be changed to a specific value for a specific flow problem. It is obvious that the theory is more general than that of the Boltzmann transformation, which is the basic foundation of the Bruce-Klute method. However, it is easy to show that general similarity theory reduces to the special case of the Boltzmann transformation when the water content of the inlet boundary is constant. The Bruce-Klute method (1956) is only a special case of the general similarity method. Thus, the general similarity method is more flexible than the Bruce-Klute method for describing soil water redistribution.

The results of this investigation suggest that general similarity theory allows a simple method of determining the water diffusivity function which may be more convenient and useful in the laboratory than any other method available currently. The general similarity method allows the inlet boundary to be variable in water content and allows the initial water content to be variable with distance. These conditions are more flexible and general than other constant boundary methods. A limitation for both the Bruce-Klute method (1956) and the Clothier et al. method (1983) is that the diffusivity value associated with the initial water content is zero no matter how high the initial water content. However, the similarity method does not give a zero diffusivity unless the water content is zero. The general similarity method is not only simpler than the current methods (e.g. Bruce-Klute method), it also removes the limitation of zero water diffusivity at the initial water content.

References

Abramowita, M., and I.A. Stegun. 1972. Handbook of Mathematical Functions. Dover Publications, Inc., New York.

Anderson, D., and K. O. Jeppson. 1984. Nonlinear two-step diffusion in semiconductors. J. Electrochem. Soc. : SOLID-STATE SCIENCE AND TECHNOLOGY. 131: 2675-2679.

Bruce, R. R., and A. Klute. 1956. The measurement of soil moisture diffusivity. Soil Sci. Soc. Am. Proc. 20: 458-462.

Blake, B. R., and K. H. Hartge. 1986. Particle density. Method of Soil Analysis. ASA monograph no. 9: 377-382.

Carter, D.L., M.M. Mortland, and W.D. Kemper. 1986. Specific surface. Method of Soil Analysis, ASA monograph no. 9: 413-423.

Cassel, D. K., A. W. Warrick, D. R. Nielsen, and J. W. Biggar. 1968. Soil-water diffusivity values based upon time dependent soil-water content distributions, Soil Sci. Soc. Am. Proc. 32: 774-777.

Chihacek, L.J., and J.M. Bremner. 1979. A simplified ethylene glycol monoethyl ether procedure for assessment of soil surface area. Soil Sci. Soc. Am. J. 43: 821-822.

Clothier, B. E., D. R. Scotter, and A. E. Green. 1983. Diffusivity and one-dimensional absorption experiments. Soil Sci. Soc. Am. J. 47: 641-644.

Hogarth, W.L., J.-Y. Parlange, and R.D. Braddock. 1989. First integrals of the infiltration equation: 2. Nonlinear conductivity. Soil Sci. 148: 165-171.

Kirkham, D., and W. L. Powers. 1972. Advanced soil physics. Wiley-Interscience, New York.

Klute, A. 1952. A numerical method for solving the flow equation for water in unsaturated materials. Soil Sci. 73: 105-116.

McBride, J. F., and R. Horton. 1985. An empirical function to describe measured water distributions from horizontal infiltration experiments. Water Resour. Res. 21: 1539-1544.

Mualem, Y. 1976. A new model for predicting the hydraulic conductivity of unsaturated porous media. Water Resour. Res. 12: 593-622.

Mualem, Y., and E. E. Dagan. 1975. A dependent domain model of capillary hysteresis. Water Resour. Res. 11: 452-460.

Parlange, J.-Y., R.D. Braddock, and B.T. Chu. 1980. First integrals of the diffusion equation: An extension of the Fujita solutions. Soil Sci. Soc. Am. J. 44: 908-911.

Parlange, J.-Y., and J.F. Fleming. 1984. First integrals of the infiltration equation: 1. Theory. Soil Sci. 137: 391-394.

Philip, J.R. 1960. General method of exact solution of the concentration-dependent diffusion equation. Aust. J. Phys. 13: 1-12.

Ross, P.J., and J.-Y. Parlange. 1994a. Investigation of a method for deriving unsaturated soil hydraulic properties from water content profiles. Soil Sci. 157: 335-340.

Ross, P.J., and J.-Y. Parlange. 1994b. Comparing exact and numerical solutions of Richards' equation for one-dimensional infiltration and drainage. Soil Sci. 157: 341-344.

Warrick, A. W. 1994. Soil water diffusivity estimates from one-dimensional absorption experiments. Soil Sci. Soc. Am. J. 58: 72-77.

Willmott, C.J., S.G. Ackleson, R.E. Davis, J.J. Feddema, K.M. Klink, D.R. Legates, and C.M. Rowe. 1985. Statistics for the evaluation and comparison of models. J. Geophy. Res. 90: 8995-9005.

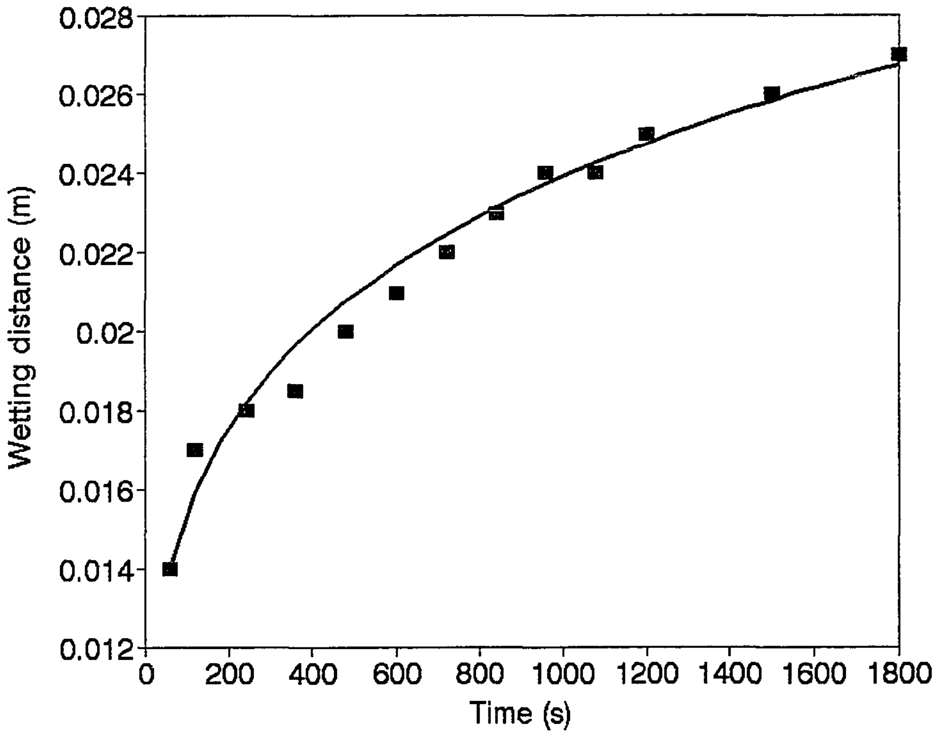

Figure 1. An example of the wetting front advance with time.

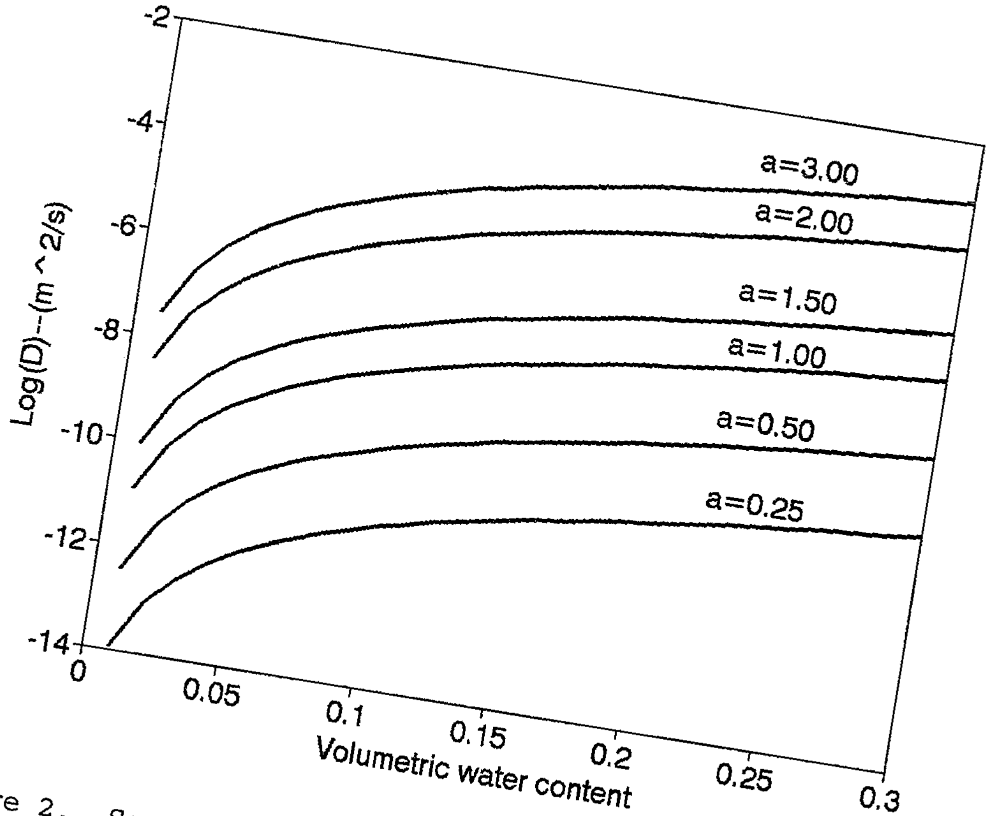

Figure 2. Sensitivity of diffusivity to parameter a (b=0.2).

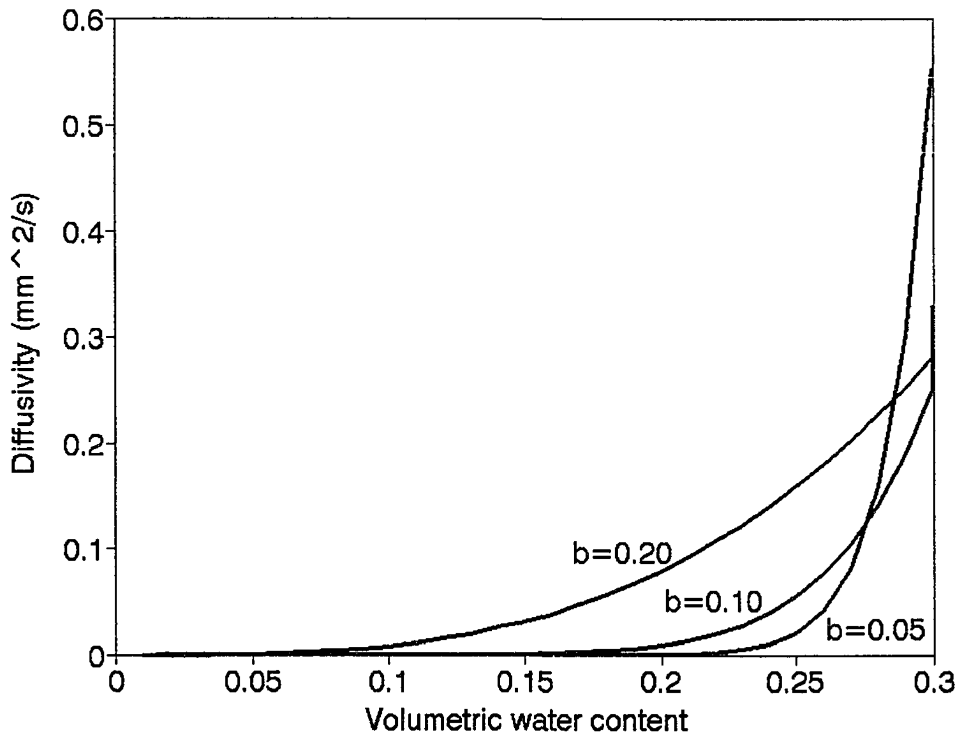

Figure 3. Sensitivity of diffusivity to parameter b (a=1).

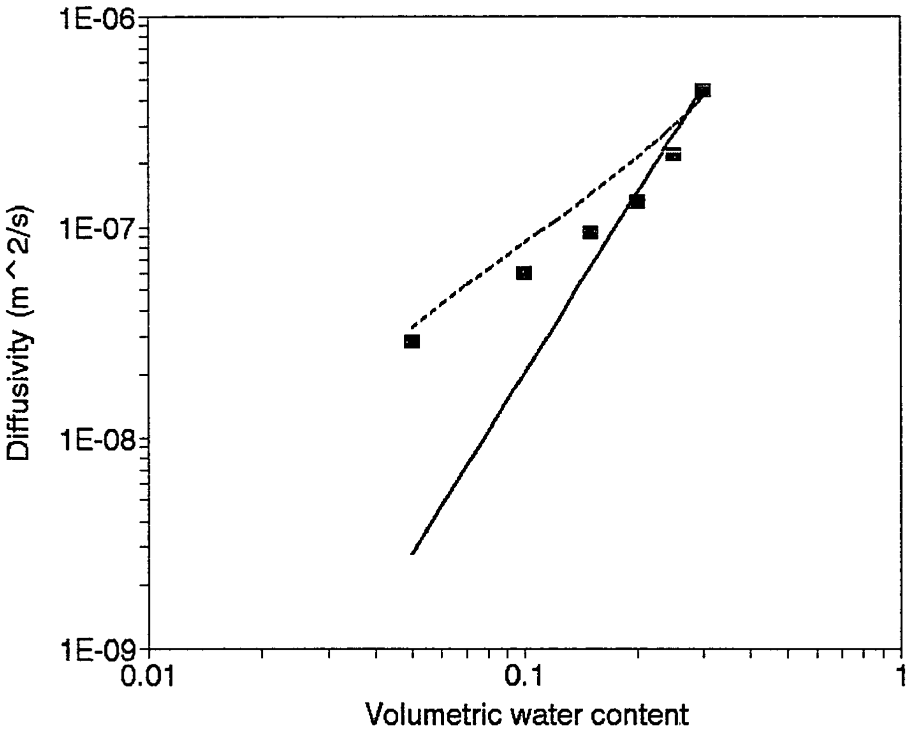

Figure 4a. Water diffusivities of sandy clay loam, filled square--by Bruce-Klute method, dashed curve--by Clothier et al method, solid curve--by general similarity.

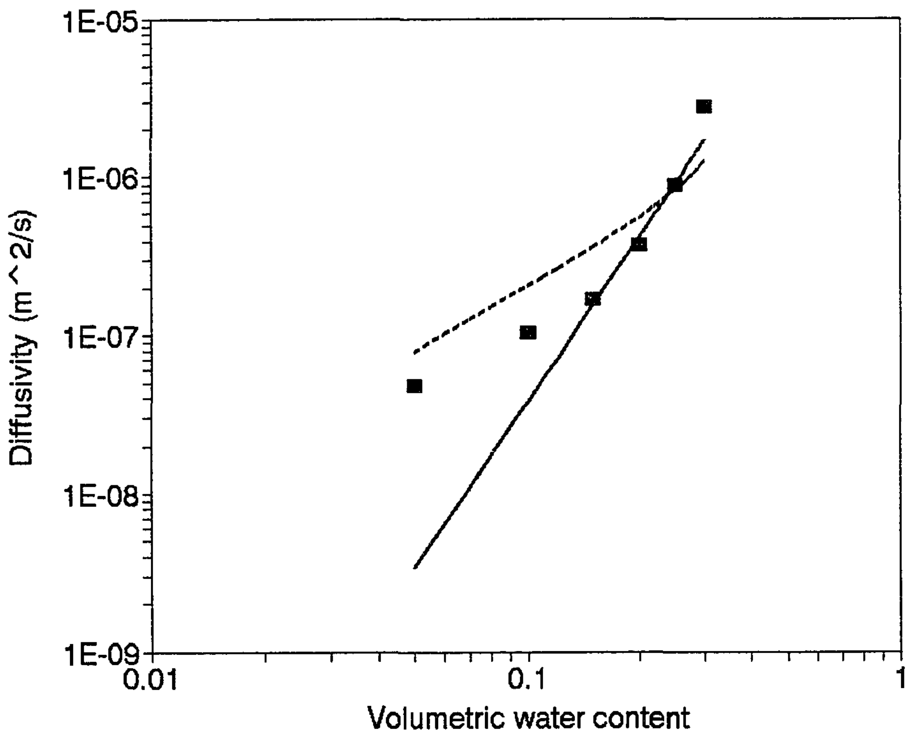

Figure 4b. Water diffusivities of loam, filled square--by Bruce-Klute method, dashed curve--by Clothier et al method, solid curve--by general similarity.

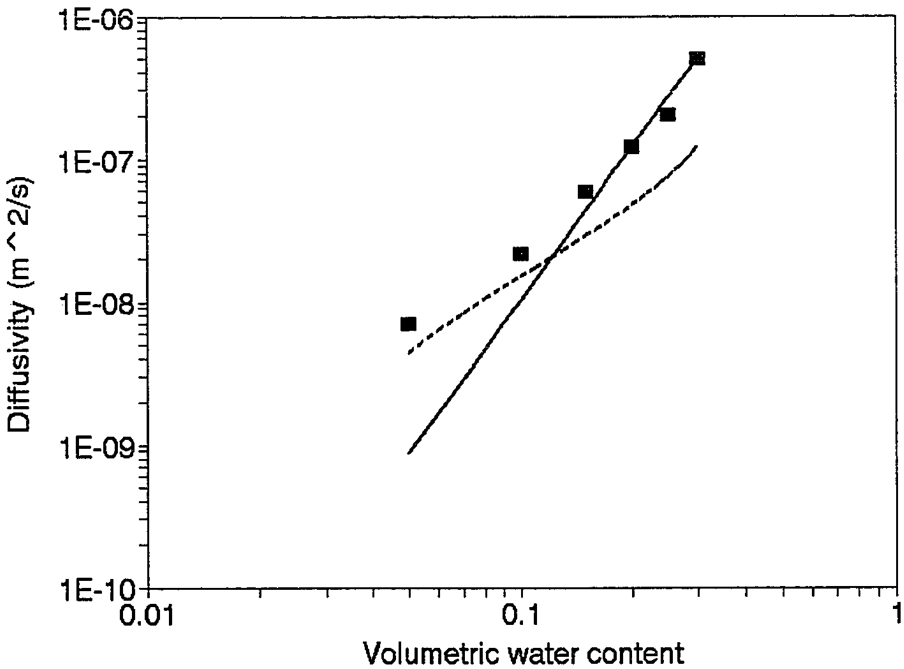

Figure 4c. Water diffusivities of silt loam, filled square--by Bruce-Klute method, dashed curve--by Clothier et al method, solid curve--by general similarity.

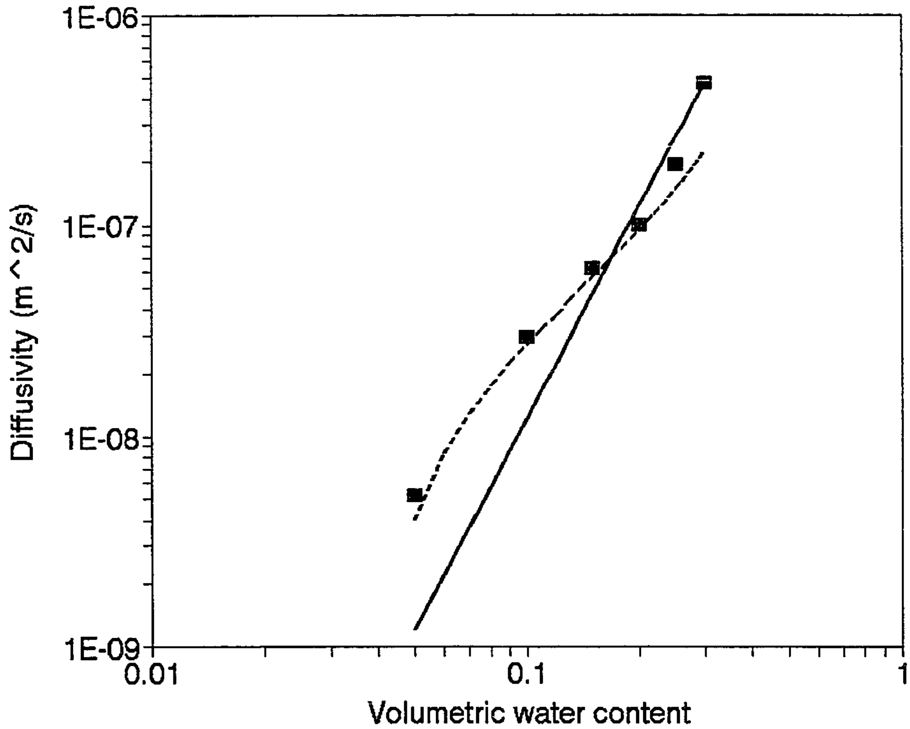

Figure 4d. Water diffusivities of silty clay loam, filled square--by Bruce-Klute method, dashed curve--by Clothier et al method, solid curve--by general similarity.

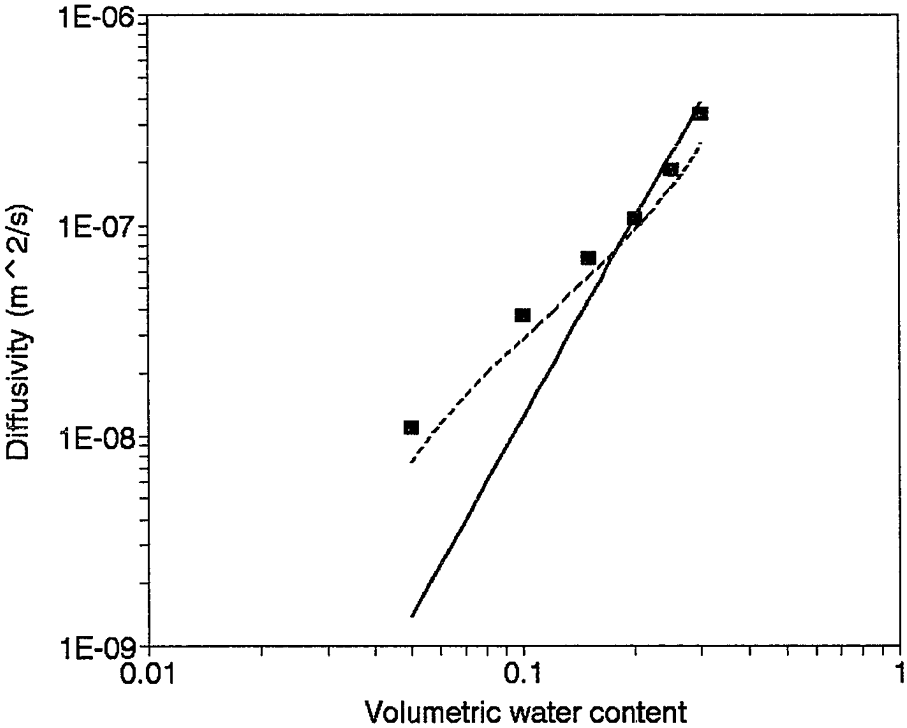

Figure 4e. Water diffusivities of clay loam, filled square--by Bruce-Klute method, dashed curve--by Clothier et al method, solid curve--by general similarity.

CHAPTER 4. EXACT SOLUTION FOR HORIZONTAL REDITRIBUTION BY GENERAL SIMILARITY

A paper to be submitted to Soil Science Society of America Journal

Mingan Shao and Robert Horton

Abstract

This paper presents an exact solution to horizontal water redistribution by using general similarity theory. A power function of soil water diffusivity is used in deriving the exact solution. The similarity solution contains initial wetted length, amount of water infiltrated, and coefficients of water diffusivity. Similarity solutions for three initial conditions are compared with corresponding numerical solutions. Error analysis indicates that the maximum global errors in water content are within 2%. General similarity theory provides an approach to exactly solve horizontal flow problem with variable first-type boundary and initial conditions while Boltzmann transformation is restricted to constant first-type boundary and initial conditions.

Introduction

The understanding and prediction of the redistribution of water which has infiltrated is just as important as those of infiltration process itself [Philip, 1991]. Redistribution determines the quantity of water stored in the root zone of crops or natural vegetation and the duration of time this water remains available for uptake by plant roots [Sander et. al., 1991]. Knowledge of water redistribution is also needed to determine whether water or solutes penetrate the root zone. Such knowledge is useful for agricultural chemical management.

This paper includes derivation of an exact solution for nonlinear, nonhysteretic redistribution of water in a horizontal soil column by using general similarity theory. The nonlinear water diffusivity used here is a power function that has been used for more than two decades by a number of soil physicists [Parlange et al., 1980; Parlange and Fleming, 1984; Ross and Parlange, 1994a and 1994b]. Philip [1991] gave an analytical solution to the redistribution of water in a horizontal column of infinite dimension. The key for his solution is the similarity character of the horizontal columns with two parts, $x<0$ and $x>0$ at uniform high and low moisture contents. He used Boltzmann transformation and assumed power-law flux-concentration relations to solve the problem. Philip's solution [1991] is an implicit integral and needs iterative numerical integrations to have sorptivity be equal to desorptivity. In our analysis, the column does not need necessarily to have similarity character, i.e., the length of the wet part can be arbitrary.

Realistic solutions of redistribution problems should take capillary hysteresis effects into account. Currently, only numerical techniques can actually incorporate hysteresis effects into water flow model. In fact, Philip's hysteretic solution [1991] to the problem is much more involved in numerical integration than his nonhysteretic solution. In other words, the hysteretic solution is technically a numerical one in terms of calculation. There is some evidence [Watson and Sardana, 1987] that the size of the hysteresis loop decreases for fine-textured soils. Nonhysteretic solutions still have applications to water redistribution of these soils.

The purpose of this paper is to improve upon existing Boltzmann transformation method by presenting an exact solution to horizontal water redistribution by using general similarity theory. Boltzmann transformation method is a specific form of the general similarity theory. This paper will also compare the exact solutions by general similarity with numerical solutions to show the capacity and reliability of the general similarity theory for different initial conditions.

Theory

The equation for one-dimensional horizontal flow is given by (Bruce and Klute, 1956)

$$\partial\theta/\partial t = \partial(D(\theta)\partial\theta/\partial x)/\partial x \qquad (1)$$

where θ is the volumetric water content (m^3/m^3), t is the time (s), x is the distance (m), and D is the soil water diffusivity (m^2/s).

The initial and boundary conditions for the horizontal redistribution are

$$\theta(x, 0) = f(x) \qquad x \le x_0 \qquad (2a)$$

$$\theta(x, 0) = \theta_i \qquad x > x_0 \qquad (2b)$$

$$q(0, t) = -D(\theta)\ \partial\theta(0, t)/\partial x = 0 \qquad (3)$$

$$\theta(x_f, t) = \theta_i \qquad (4)$$

in which x_0 is the length of the wet part of the horizontal flow system, f(x) is the water content distribution of the wet part water (if the water content is uniform then f(x) is a constant), θ_i is the initial water content in the dry part, q(0, t) is the flux density at the zero-position boundary, and x_f is the position of the wetting front. Water is redistributed from the wet part to the dry part and no water flows in and out of the system.

Simplifying assumptions are needed to solve the nonlinear flow equation analytically for this particular flow problem. First of all, we adopt the power function of the water diffusivity, i.e.:

$$D(\theta) = D_0\ \theta^{\gamma} \qquad (5)$$

where D_0 and γ are constants.

For the sake of simplicity, let θ_i = constant, and particularly let $\theta_i = 0$ (water redistribution into an oven-dry soil). This assumption was also used in solving the diffusivity equation by Parlange et. al. (1980). With these assumptions, the problem can be reduced as follows:

$$\partial\theta/\partial t = \partial(D_0\theta^\gamma\ \partial\theta/\partial x)/\partial x \qquad 0 < t\ ,\ 0 < x < \infty \tag{6}$$

$$\theta(x,\ 0) = 0 \qquad x_0 < x < \infty \tag{7}$$

$$\partial\theta(0,\ t)/\partial x = 0 \qquad 0 < t \tag{8}$$

$$\theta(x_f,\ t) = 0 \qquad 0 < t \tag{9}$$

By introducing $\tau = D_0\ t$, then (6) is normalized as

$$\partial\theta/\partial\tau = \partial\ (\theta^\gamma\ \partial\theta/\partial x)/\partial x \tag{10}$$

By using general similarity, the solution to (10) is written as

$$\theta = \tau^\alpha\ \phi(\xi) \tag{11}$$

$$\xi = x/\tau^\beta \tag{12}$$

Inserting (11) and (12) into (10), we find that the power of τ matches only if α and β are related by

$$\alpha = (2\beta - 1)/\gamma \tag{13}$$

and the resulting equation for $\phi(\xi)$ is then

$$\alpha\phi - \beta\xi \; d\phi/d\xi = d/d\xi \; (\phi^{\gamma} \; d\phi/d\xi) \tag{14}$$

According to the mass balance, i.e.:

$$\int_0^{\infty} \theta(x,\tau)dx = \tau^{\alpha+\beta} \int_0^{\infty} \phi(\xi) \; d\xi = H_0 \tag{15}$$

where H_0 is the amount of water in the wet part (m), of course, H_0 is a constant.

(15) obviously requires $\alpha = -\beta$, which, together with relation (13), determines α and β to be

$$\alpha = -\beta = -1/(2 + \gamma) \tag{16}$$

With α and β given by (16), (14) can be integrated explicitly to yield

$$\phi(\xi) = \phi_0 \; (1 - \xi^2/\xi_f^{\,2})^{1/\gamma} \tag{17}$$

in which the characteristic wetting depth, ξ_f, is related to the integration constant, ϕ_0, by

$$\xi_f^2 = 2\phi_0^\gamma \ (2 + \gamma)/\gamma \tag{18}$$

Furthermore, the integration constant, ϕ_0, is determined by

$$\phi_0 = (H_0^2 \ \gamma/(2(2 + \gamma)I_\gamma^2))^{1/(2+\gamma)} \tag{19}$$

where I_γ is an integration constant.

Combining (18) and (19), ξ_f is obtained as

$$\xi_f = (2H_0^\gamma(2 + \gamma)/(\gamma I_\gamma^\gamma))^{1/(2+\gamma)} \tag{20}$$

and the wetting front, x_f, is written as

$$x_f(\tau) = (2(2 + \gamma)H_0^\gamma \ \tau/(\gamma I_\gamma^\gamma))^{1/(2+\gamma)} \tag{21}$$

Then, the solution to the original wetting front, $x_f(t)$, is

$$x_f(t) = (2(2 + \gamma)H_0^\gamma \ D_0 t/(\gamma I_\gamma^\gamma))^{1/(2+\gamma)} \tag{22}$$

From (22), it is obvious that D_0 and γ can be obtained by fitting (22) to observed wetting front data. With D_0 and γ soil water diffusivity can be estimated by using equation (5).

Collecting our results, we find that $\theta(x,t)$ can be written as:

$$\theta(x,\tau)=\theta_0(\tau)\,(1-(x/x_f)^2)^{1/\gamma} \tag{23}$$

$$\theta_0(\tau)=((\gamma H_0^2)/(2(2+\gamma)I_\gamma^2\tau)^{1/(\gamma+2)} \tag{24}$$

where $\theta_0(t)$ is a decaying maximum water content at x=0. Equations of (21), (23), and (24) complete the analytical solution to this problem. The only step remaining is to incorporate the feature of a finite length of the wet part of the soil column. This can be done by relating the initially wetted length of the column with an arbitrarily constant time (τ_0). Then a more general similarity solution that incorporates the initial wetted length is obtained through arbitrary time translations of the previous solution because Eq. (10) is invariant under such time translations, i.e.:

$$\theta(x,\tau)=\theta_s(\tau+\tau_0)\,(1-(x^2/x_f^2(\tau+\tau_0))^{1/\gamma} \tag{25}$$

From Eq.(12), the arbitrary time constant, τ_0, can be related to the length of the wet part, x_0, infiltrated water, H_0, and water diffusivity coefficient, γ, by the following expression:

$$\tau_0=(x_0/\xi_f)^{\gamma+2}=\gamma/(2(\gamma+2))\;\;(I_\gamma/H_0)^\gamma\;x_0^{\gamma+2} \tag{26}$$

With Eq.(21), (25), and (26), the general similarity solution to the redistribution problem of soil water is complete. In the following part of this paper, the general similarity solution is compared to a numerical solution for different initial conditions. Our numerical solution is obtained by using CSMP (the Continuous System Modeling Program). CSMP is a program especially designed to allow users to simulate all types of physical systems with a minimum of programming [Speckhart and Green, 1976].

Results and Discussion

1. Water Redistribution within a Two-Part Column

First, a simple initial condition will be considered, i.e., the profile of initial water content is a step function. This represents the redistribution of soil water in a two-part soil column. One part of the column is uniformly wet, the other part is uniformly dry. Physically, one column is wetted and then connected with a dry soil column. The water redistribution in the combined column is the problem in our consideration. This initial condition is shown in Fig. 1.

The coefficients of water diffusivity were taken to be D_0=0.12 cm^2/min, and γ=0.71. The comparison of the decaying maximum water contents, $\theta_0(t)$, at x=0 cm is shown in Fig. 2. The general similarity (referred as analytical) $\theta_0(t)$ is in very good agreement with the numerical one (referred as CSMP). This indicates that the left boundary water content (wetted boundary) can be well predicted by the analytical solution.

The comparison of soil water profiles obtained from general similarity theory and the numerical solution is shown in Fig. 3. From Fig. 3, we can see that at anytime the two water content profiles obtained by general similarity theory and by the numerical solution are almost the same. We can also note that the area under each curve is the same, i.e., both the analytical and numerical solutions behave well in accordance with mass conservation law because the infiltrated amount of water (the area) is given (0.63 cm).

In Fig. 4, the global error in water content as described as the difference between numerical solution and similarity solution is illustrated. The error is small and decreases with time. This indicates that the general similarity solution has the ability to predict water redistribution not only for short time but also for long time. Long time prediction of water redistribution by numerical solution usually needs more computing time. The general similarity solution overcomes this limitation from numerical solution. The maximum error for the time concerned is within 0.003. The maximum error for a specific time happens at the wetting front. The wetting front zone of redistribution is the most difficult part to predict by using numerical solutions.

2. Redistribution within a Column with Similarity Initial Condition

In this section, a flow system similar to the one described above part is used. Here the water content profile after 10 minutes of redistribution is used as the initial condition (referred to similarity initial condition). The similarity initial condition is shown in Fig. 5. The comparison of water content profiles between similarity theory and numerical solution is shown in Fig. 6. Fig. 6 gives evidence that the general similarity solution is not only good for the initial condition of a step function but also good for a similarity initial condition. This implies that the general similarity solution can predict water redistribution of the experimental condition where water infiltrates into a soil column and then infiltration is stopped while redistribution occurs.

3. Redistribution within a Column after Infiltration

The final case considered in this paper is the redistribution problem of soil water after infiltration. Experimentally, water first infiltrates into a soil column, infiltration ceases, and the inlet boundary is closed while water redistributes. The initial condition is presented in Fig. 7. The zero water content (corresponding to oven-dried soil) of the dry part of previous cases has been altered to a non-zero water content (corresponding to air-dried soil). One of the measured water content profile of diffusivity determination by Bruce-Klute (1956) method was selected as the initial condition. The length of the column was changed from 10 cm to 40 cm. In Fig. 8, we show a comparison of water content profiles between similarity prediction and numerical solution. In this case the predictability of the general similarity for water redistribution is still good. The maximum error is within 0.02. This error is from the approximation of the initial condition. In this case only two parameters, the wetted length (X_0) and the amount of infiltrated water (H_0), are used to describe the initial water content profile in the general similarity solution. This may introduce an error especially for early time.

Conclusions

General similarity solutions for redistribution of soil water with certain restrictive boundary condition but flexible initial conditions and general soil flow properties (D_0 and γ can be chosen arbitrarily) have been presented. The general similarity solutions are closed form and flexible. Similarity solutions for three initial conditions compare well with the corresponding numerical solutions. The similarity solution itself provides a method of estimating soil water diffusivity. This method only requires an experimentalist observe the advance of wetting front with time during a water redistribution experiment to estimate soil water diffusivity.

References

Bruce, R. R., and A. Klute. 1956. The measurement of soil moisture diffusivity. Soil Sci. Soc. Am. Proc. 20: 458-462.

Parlange, J.-Y., R.D. Braddock, and B.T. Chu. 1980. First integrals of the diffusion equation: An extension of the Fujita solutions. Soil Sci. Soc. Am. J. 44: 908-911.

Parlange, J.-Y., and J.F. Fleming. 1984. First integrals of the infiltration equation: 1. Theory. Soil Sci. 137: 391-394.

Philip, J.R. 1991. Horizontal redistribution with capillary hysteresis. Water Resour. Res. 27(7): 1459-1469.

Ross, P.J., and J.-Y. Parlange. 1994a. Investigation of a method for deriving unsaturated soil hydraulic properties from water content profiles. Soil Sci. 157: 335-340.

Ross, P.J., and J.-Y. Parlange. 1994b. Comparing exact and numerical solutions of Richards' equation for one-dimensional infiltration and drainage. Soil Sci. 157: 341-344.

Speckhart, F.H., and W.L. Green. 1976. A guide to using CSMP-the Continuous System Modeling Program. Prentice-Hall, Inc., Englewood Cliffs, New Jersey.

Vachaud, G, and J.-L. Thony. 1971. Hysteresis during infiltration and redistribution in a soil column at different initial water contents. Water Resour. Res. 7(1): 111-127.

Watson, K.K., and V. Sardana. 1987. Numerical study of the effect of hysteresis on post infiltration redistribution, paper presented at the International Conference of

Infiltration Development and Application in Hawaii, University of Hawaii, Jan. 6-9.

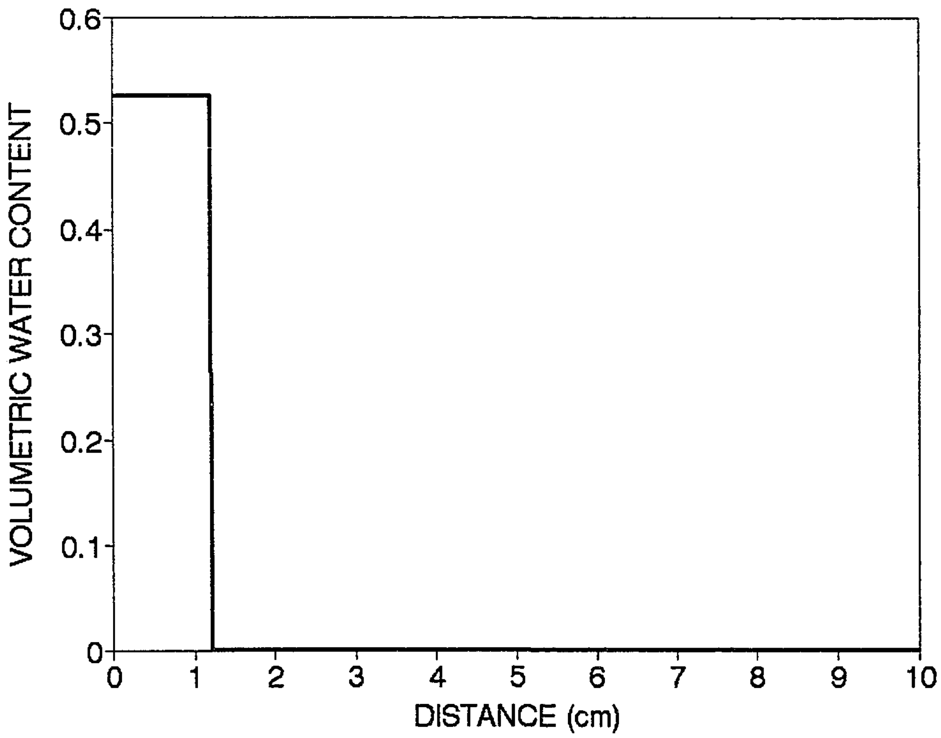

Figure 1. The initial condition of water redistribution within a two-part column.

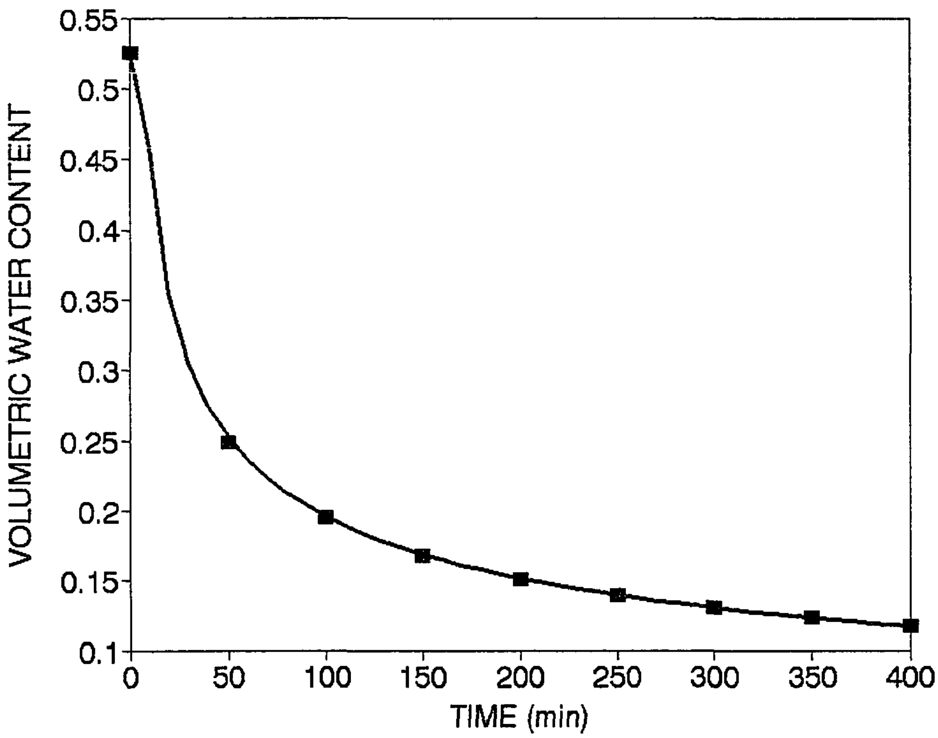

Figure 2. The comparison of the decaying maximum water contents, filled square--numerical prediction and solid curve-- analytical prediction.

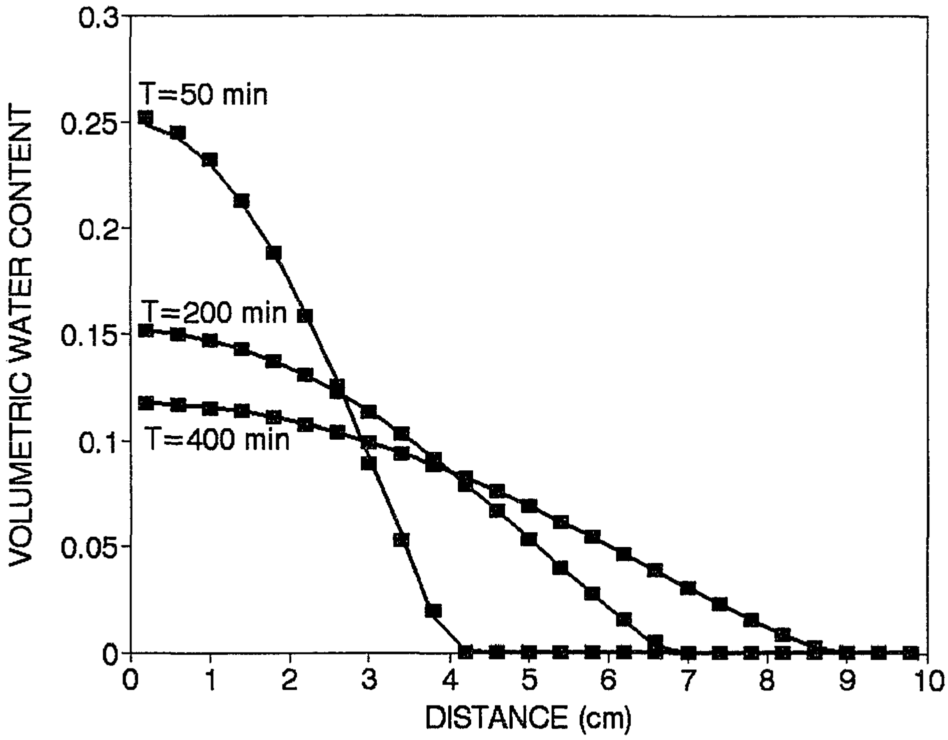

Figure 3. The comparison of soil water content profiles predicted by analytical solution (solid curve) and numerical solution (filled square) for a two-part soil column.

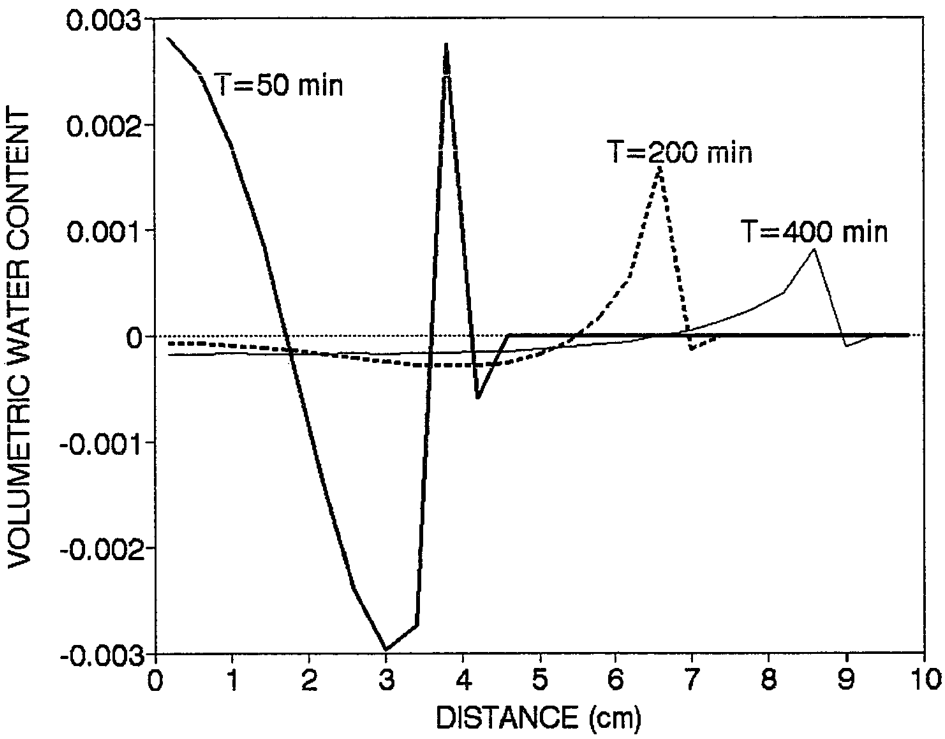

Figure 4. Global error distribution for water redistribution in a two-part soil column.

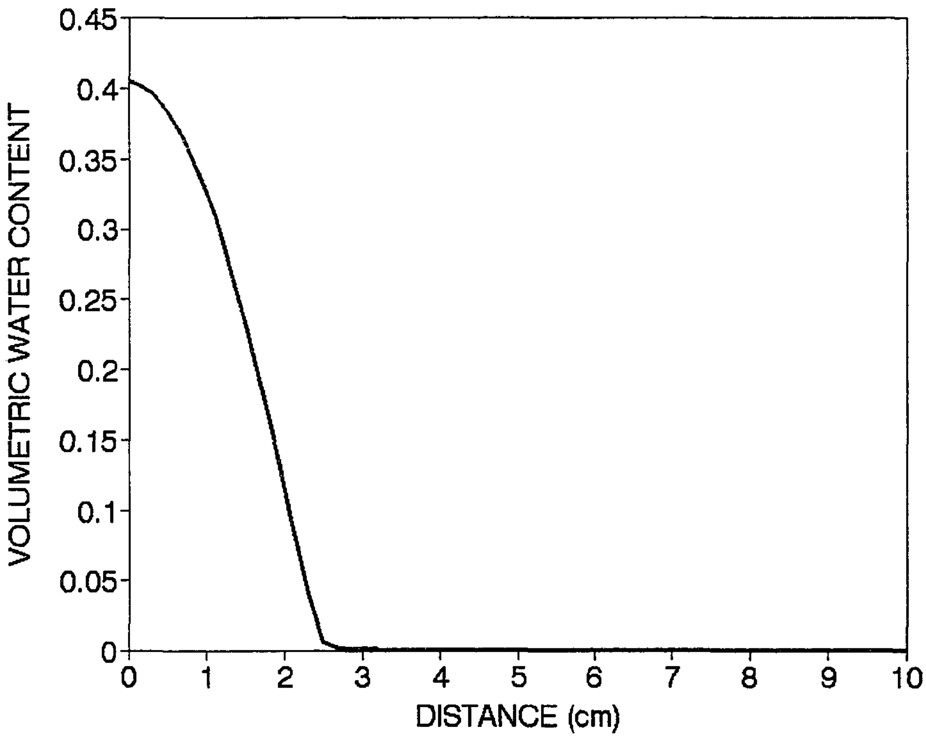

Figure 5. Similarity initial condition.

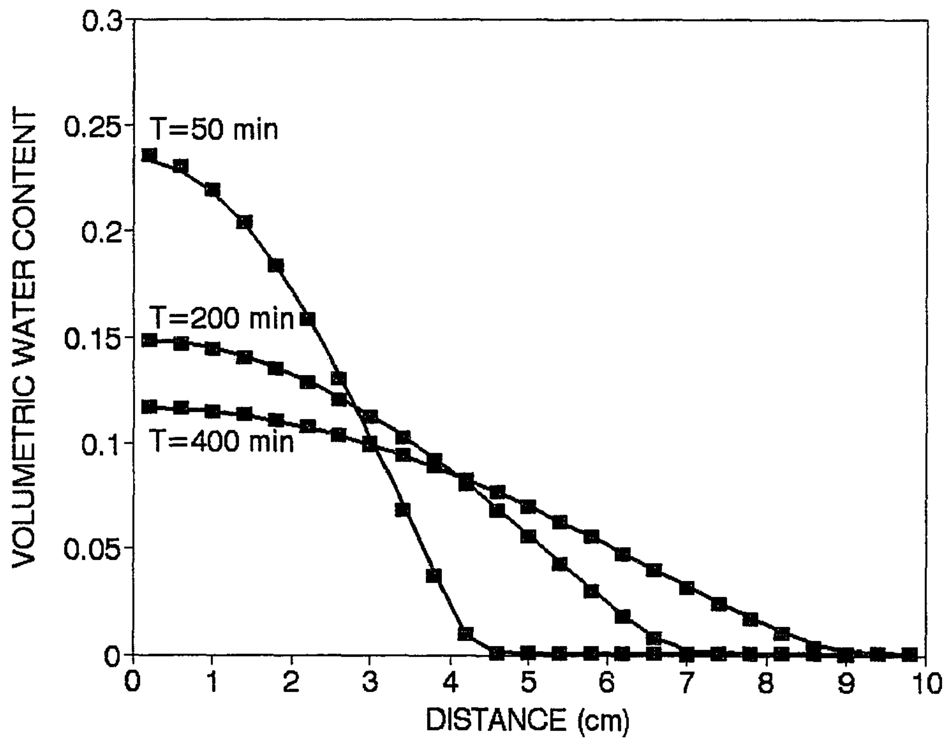

Figure 6. The comparison of soil water content profiles predicted by analytical solution (solid curve) and numerical solution (filled square) for water redistribution with a similarity initial condition.

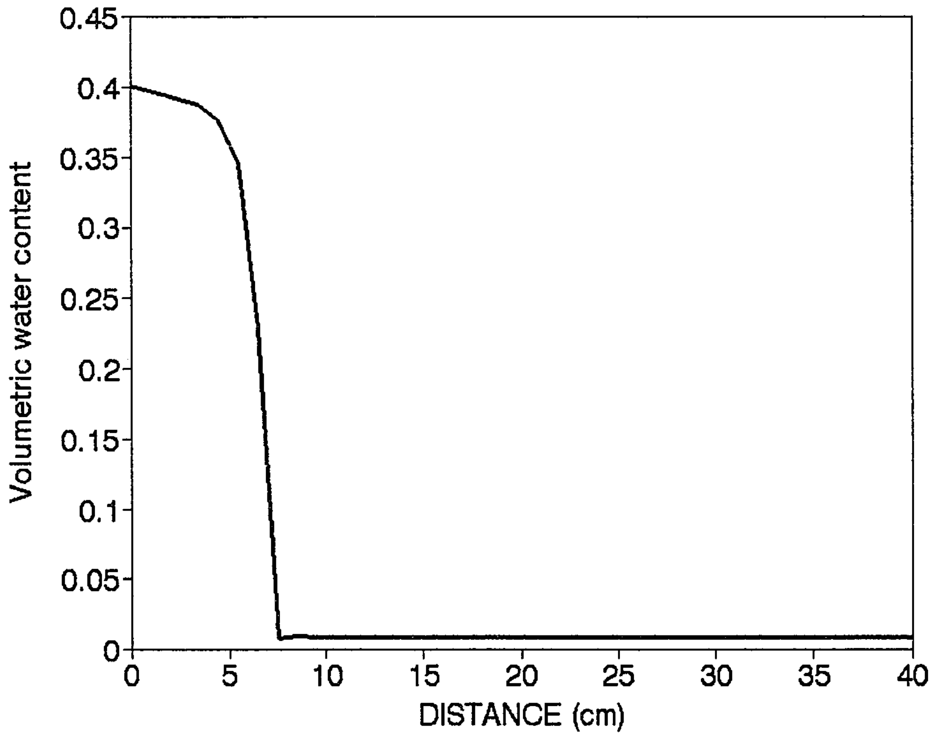

Figure 7. The initial condition of redistribution after infiltration.

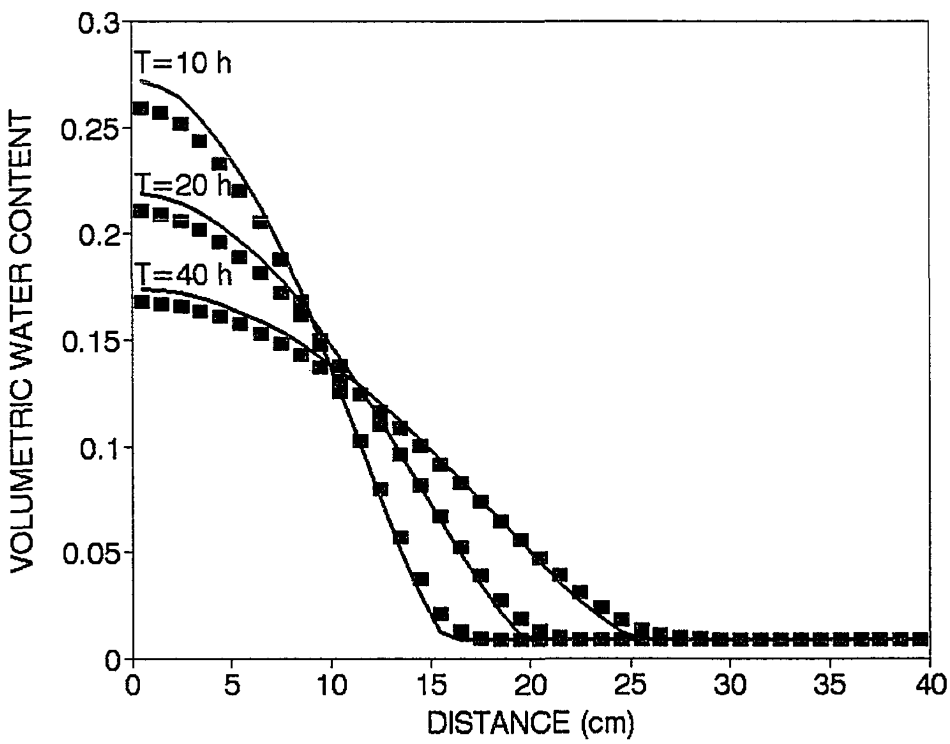

Figure 8. The comparison of soil water content profiles predicted by analytical solution (solid curve) and numerical solution (filled square) for water redistribution after infiltration.

CHAPTER 5. SIMPLE WATER INFILTRATION METHOD FOR ESTIMATING SOIL HYDRAULIC PROPERTIES: I. THEORETICAL ANALYSIS

A paper to be submitted to Soil Science
Society of America Journal

Mingan Shao and Robert Horton

Abstract

Knowledge of soil hydraulic properties is required to fully understand and predict water distribution. Soil hydraulic properties include soil characteristic curve and hydraulic conductivity. In this paper an integral method is used to solve the problem of water absorption into a horizontal soil column. The integral solutions to the problem are used to estimate the parameters, α and n, in the van Genuchten model of a soil characteristic curve. The two parameters, α and n, in the characteristic curve model are estimated by the length of wetted zone, sorptivity, and saturated hydraulic conductivity. Unsaturated soil hydraulic conductivity is then estimated from the parameters determined in the soil characteristic curve. This new integral method uses both Richards' equation and the closed form equations of soil hydraulic properties. The integral method provides a transient water flow approach to estimate the soil

characteristic curve instead of the usual equilibrium method. This is a new and simple means to determine soil hydraulic properties.

Introduction

Increasing evidence shows that the quality of soil and water resources on the Earth is being adversely affected by the release of a variety of agricultural and industrial pollutants into the environment (van Genuchten, 1992). Water is the most important carrier of the pollutants into our soils. Rates of soil water movement in various soil flow processes (e.g., infiltration, redistribution, root uptake, and drainage)are important for making practical soil management decisions to minimize potential groundwater contamination and degradation of soil quality from land applied chemicals. Numerical solutions of the flow and transport problems in the vadose zone are the most important approaches to predict quantitatively the dynamic behavior of the system. Unsaturated flow and transport modeling usually requires accurate and complete information about the unsaturated hydraulic properties for the model to function properly. The methods of determining unsaturated hydraulic properties are conveniently divided into two groups, i.e., direct methods and indirect methods (Neuman, 1973; van Genuchten, 1992).

For the direct group, most methods for measuring soil hydraulic properties, i.e., soil water retention characteristics and hydraulic conductivity, both in the laboratory and in situ, have been described by Green et al. (1986) and by Klute and Dirksen (1986), respectively. Although direct methods are relatively clear in concept, they have some limitations that restrict their use in practice (van Genuchten, 1992). The time required and uncertainty in estimating hydraulic parameters are the common limitations for most direct methods, especially for field methods.

Because the direct determination of hydraulic properties is relatively time consuming and expensive, various efforts have been made to relate hydraulic conductivity and water retention characteristic curve to easily determined soil physical properties. This approach results in indirect methods (also referred to as parameter estimation methods). For example, soil texture data were successfully used (Puckett et al., 1985; Dane and Puckett, 1992; Tyler and Wheatcraft, 1989 and 1990) to predict the water retention curves, which could subsequently be used to estimate the hydraulic conductivity based on the models of Brooks and Corey (1964), Mualem (1976), and van Genuchten (1980). Recent application of indirect methods (Kool et al., 1987; Kool and Parker, 1988; Russo et al., 1991; Sisson and van Genuchten, 1991; Arya and Dierolf, 1992; Wu and Vomocil 1992) have shown several advantages of indirect methods compared with the direct techniques (van Genuchten, 1992). Complete hydraulic property estimation over a wide range of soil water content and information about parameter uncertainty are major advantages of indirect methods. A number of problems, however, such as convergence and parameter uniqueness, related to indirect methods still remain to be solved (van Genuchten, 1992).

To remove limitations both from direct methods and indirect methods, this paper will present an integral method for estimating soil hydraulic properties. The integral method is theoretically based on Richards' equation of water flow in soils, and it is practical, easy, and convenient to determine the required parameters. The integral method gives approximate solutions to nonlinear partial differential equations (PDE). The essential idea of the integral method is to approximate the solution to PDE with some simple function that contains adjustable parameters, and then determine the values of these parameters by requiring the solution to satisfy both the PDE and initial and boundary conditions in an integral sense. The integral method was first used to solve diffusion problems by Landahl (1953). There have been applications of this method in flow problems of porous media (Prasad and Romkens, 1982; Zimmerman and Bodvarsson, 1989; Zimmerman et al., 1990). This paper illustrates how the integral approach can be used to solve the highly nonlinear horizontal flow equation of soil and how to estimate the parameter values of the van Genuchten (1980) hydraulic property models.

Theory

The equation describing one-dimensional horizontal unsaturated flow of water in unsaturated soils is

$$\frac{\partial \theta}{\partial t}=\frac{\partial}{\partial x}[K(h)\,\frac{\partial h}{\partial x}] \tag{1}$$

where θ is the volumetric soil water content (m^3/m^3), h is the pressure head (m), K(h) is the unsaturated conductivity (m/s), x is the horizontal distance (m), and t is the time (s).

The initial and boundary conditions are similar to those of the Bruce-Klute (1956) water absorption problem. The only difference is that the variable to describe the initial and boundary conditions in Bruce-Klute (1956) water absorption is water content, and the variable in this research is pressure head. Mathematically, they are described as follows:

$$h(x,0)=h_i \tag{2}$$

$$h(0,t)=0 \tag{3}$$

$$h(\infty,t)=h_i \tag{4}$$

where h_i is the initial pressure head. Without loss of generality, a zero head of inlet boundary is assumed because the solution for nonzero boundary is related in a simple way

(Philip, 1957) to the solution of zero inlet boundary. Boltzmann transformation, $\lambda=x/t^{1/2}$, is used to convert the PDE, equation (1), into an ordinary differential equation (ODE). After the Boltzmann transformation, equation (1) is transformed into

$$\frac{d}{d\lambda}[K(h)\frac{dh}{d\lambda}]+\frac{\lambda}{2}\frac{d\theta}{d\lambda}=0 \tag{5}$$

The initial and boundary conditions (equation (2)-(4)) are converted to

$$h(0)=0 \tag{6}$$

$$h(\infty)=h_i \tag{7}$$

By performing the transformation, the mixed problem of PDE (equations (1)-(4)) is reduced to a two-point ODE boundary value problem, given by equations (5)-(7). In equation (5), there are two variables, h and θ; an additional equation (the soil characteristic curve) that relates the two variables is needed to solve the two-point ODE boundary value problem.

The most commonly-used closed-form equations for characterizing soil characteristic curve and hydraulic conductivity in soil physics are those of van Genuchten (1980) and Mualem (1976). The equations are

$$\theta=\theta_r+(\theta_s-\theta_r)\,[1+(\alpha|h|)^n]^{-m} \tag{8}$$

$$K(h)=\frac{K_s[1-(\alpha|h|)^{n-1}(1+(\alpha|h|)^n)^{-m}]^2}{[1+(\alpha|h|)^n]^{\frac{m}{2}}} \tag{9}$$

where $\theta(h)$ is volumetric water content, a function of pressure head; θ_s is saturated water content; θ_r is the residual water content; and α is a scaling parameter that is inversely proportional to the mean pore diameter; $1/\alpha$ is similar to air-entry pressure in the Brooks-Corey model (1964, 1966); n is the water retention curve index (shape parameter of the curve) or the pore size distribution index; K_s is the saturated hydraulic conductivity; and m=1-1/n.

An appropriate water content profile, $\theta(\lambda)$, may be obtained by the following reasoning. The flux of water infiltrating into the soil is finite. That means $dh/d\lambda$ must be finite at $\lambda=0$. It is convenient to express the relationship, $h(\lambda)$, in terms of MacLaurin's series, i.e.,

$$h=a_0+a_1\lambda+a_2\lambda^2+\ldots+\ldots \tag{10}$$

Because h(0)=0, this means $a_0=0$, then $h=a_1\lambda+\ldots+\ldots$, a_1 is a negative constant. Again h_0 is usually negative. For convenience, let $b_1=-a_1$, then b_1 is a positive constant.

Substitute this into equation (8) to take the first order approximation

$$\frac{\theta-\theta_r}{\theta_s-\theta_r}=1-m(\alpha b_1\lambda)^n \tag{11}$$

The length of wetted zone is denoted by d (see Fig. 1). To find b_1, we use the condition at $\lambda=d$, $\theta(d)=\theta_i$, so the term mb_1^n is given by

$$mb_1^n=\frac{\theta_s-\theta_i}{(\theta_s-\theta_r)(\alpha d)^n} \tag{12}$$

Combining equations (11) and (12) gives the appropriate water content profile (also see Fig. 1):

$$\theta(\lambda)=\theta_s-(\theta_s-\theta_i)\left(\frac{\lambda}{d}\right)^n, \qquad 0<\lambda<d \tag{13}$$

$$\theta(\lambda)=\theta_i, \qquad d\le\lambda<\infty \tag{14}$$

Equation (13) describes an absorption profile exactly the same as the one described by the function (Philip, 1960; Table 1, no. 2)

$$\lambda(\Theta)=\varepsilon(1-\Theta)^p, \qquad p>0; \tag{15}$$

where θ is normalized volumetric water content, $(\theta-\theta_i)/(\theta_s-\theta_i)$; ϵ is the maximum value of λ, the same as d in equation (13); and p is the slope factor. If p=1/n, one can verify that equation (13) and (15) are identical. This provides evidence that the water content profile described by equations (13) and (14) is appropriate. Equation (13) will also be verified by experimental evidence.

The maximum value of the Boltzmann variable or characteristic wetting length, d (wetting length for short), can be related to the parameters of van Genuchten's (1980) model by integrating equation (5) from λ=0 to λ=∞, with equations (13) and (14) substituted for $\theta(\lambda)$. The first term in Equation (5) is

$$\int_0^\infty \frac{d}{d\lambda}\left[K(h)\frac{dh}{d\lambda}\right]d\lambda = \left[K(h)\frac{dh}{d\lambda}\right]\Big|_0^\infty = b_1 K_s \tag{16}$$

From equation (12) b_1 is expressed as

$$b_1 = \frac{1}{\alpha d}\left[\frac{(\theta_s-\theta_i)}{m(\theta_s-\theta_r)}\right]^{\frac{1}{n}} \tag{17}$$

Equation (16) is obtained based on dh/dλ=0 at λ=∞, and $dh/d\lambda=-b_1$ at λ=0.

The second term is

$$\int_0^{\infty} \frac{\lambda}{2} \frac{d\theta}{d\lambda} d\lambda = \int_0^{d} \frac{\lambda}{2} \frac{d\theta}{d\lambda} d\lambda = \frac{-n(\theta_s-\theta_i)\,d}{2(n+1)} \qquad \textbf{(18)}$$

Again, equation (18) is obtained because the integral is zero in the interval (d,∞) and $d\theta/d\lambda$ is zero in this interval.

Combining equations (16), (17), and (18) with (5) gives

$$\alpha = \frac{2(n+1)K_s}{n(\theta_s-\theta_i)\,d^2} \left[\frac{1}{m}\left(\frac{\theta_s-\theta_i}{\theta_s-\theta_r}\right)\right]^{\frac{1}{n}} \qquad \textbf{(19)}$$

From equation (19), the scaling parameter, α, is related not only to d but also to K_s and n. To estimate both α and n, one more relation is needed if K_s is available (usually K_s is measured). This is obtained by applying Darcy's flux equation to the horizontal absorption. At x=0 (the inlet boundary), the water flux is expressed as

$$q = -\left(K(h)\frac{\partial h}{\partial x}\right)\Big|_{x=0} \qquad \textbf{(20)}$$

and

$$\frac{\partial h}{\partial x}\Big|_{x=0} = \left(\frac{dh}{d\lambda}\right)\Big|_{\lambda=0}\left(\frac{\partial \lambda}{\partial x}\right)\Big|_{x=0} \qquad \textbf{(21)}$$

From equation (10), one can get

$$\frac{dh}{d\lambda}\Big|_{\lambda=0}=a_1=-b_1 \tag{22}$$

Considering $K(h)=K_s$ at $x=0$ and the definition of Boltzmann variable and combining equations (20), (21), and (22) gives

$$q=K_s b_1 t^{-1/2} \tag{23}$$

For horizontal infiltration, if one uses Philip's two term equation the infiltration rate or flux density is given by

$$q=\frac{S}{2t^{1/2}} \tag{24}$$

where S is sorptivity that can be relatively easily obtained by analyzing the infiltration rate with time (a simple regression will find S by using equation (24)). Combining equations (17), (23), and (24) gives

$$\alpha=\frac{2K_s}{Sd}\left[\frac{1}{m}\left(\frac{\theta_s-\theta_i}{\theta_s-\theta_r}\right)\right]^{\frac{1}{n}} \tag{25}$$

Comparing equation (19) with (25) gives an estimation of n as

$$n=\frac{S}{d(\theta_s-\theta_i)-S} \tag{26}$$

Equations (19) and (26) complete the parameter estimation for the van Genuchten (1980) model of hydraulic properties of a soil. First, n is obtained by measuring the characteristic wetting length and sorptivity. Then, with a K_s measurement, the scaling parameter, α, is found by using equation (19). Experimentally, if one records both infiltration and wetting front with time in a horizontal absorption experiment and measures the saturated hydraulic conductivity of the column after absorption, the parameter estimation for the van Genuchten model (1980) can be completed because saturated and residual water content are easy to measure or estimate.

Discussion

Equations (19) and (26), representing the parameter estimation of the van Genuchten model (1980) of soil hydraulic properties, depend on six parameters, K_s, S, d, θ_s, θ_r, and θ_i. The two water contents, θ_s and θ_i, are easy to measure as the infiltration and initial conditions, respectively. θ_r needs to be estimated (for example taking the water content at -15 bar pressure potential as θ_r). The characteristic length (d) of wetted zoned is easy to observe visually during infiltration. S is also relatively easy to determine from infiltration data. The only parameter left to determine is the saturated hydraulic conductivity (K_s). K_s can be conveniently measured by using the same soil column after the absorption experiment.

Equation (13) is used to derive the two equations, (19) and (26). As mentioned before equation (13) is approximate. Equations (13) and (15) are identical. Equation (15) should cover most absorption profiles of soil water content (Clothier et al., 1983). However testing of equation (13) by observed data of water content distribution profiles should be performed. In order to test equation (13) observed data for ten soils ranging from sand to clay were taken from the literature. The ten soils are: Hagener sand (Selim et al., 1970), Hayden sandy loam (Whisler et al., 1968), Manawatu fine sandy loam (Clothier et al., 1983), Adelanto loam (Jackson, 1963), Edina silt loam (Selim et al., 1970), Nicollet sandy clay loam (McBride and Horton, 1985), Fayette silty clay loam (McBride and Horton, 1985), Panoche clay loam (Reichardt et al., 1972), Pine silty clay (Jackson, 1963), and Yolo clay (Nofziger, 1978). Figure 2 (from Fig. 2a to Fig. 2j) presents the fit of equation (13) to water distribution data for these ten soils. Figure 2 provides evidence that equation (13) is appropriate for describing soil water distribution of a horizontal absorption experiment.

In the derivation of equations (19) and (26), equation (13) is the only approximate expression. In fact its derivative (not equation (13) itself) is used in order to integrate the second term of equation (5). Both theoretical and experimental verifications of equation (13) give confidence that equations (19) and (26) should be appropriate for parameter estimations of the van Genuchten model (1980) of a soil characteristic curve.

Equation (19) should be examined carefully. For a given soil, K_s, d, θ_s, θ_r, and θ_i are constant. Therefore it is obvious that the scaling parameter, α, is related to the shape parameter, n. The relationship is shown in Fig. 3. Figure 3 shows that α increases with the increase of n. In other words for given soil conditions an overestimation of n will result in an overestimation of α. This means an error in estimating one parameter will introduce an error to the other parameter.

The shape parameter, n, in the van Genuchten model (1980), is related both to sorptivity (S) and the characteristic length (d) of the wetted zone. Clothier and Scotter (1982) provided experimental evidence that the relationships, $\theta(\lambda)$, for several times overlapped. In other words, d is a constant for a given soil. That means that d is an indicator of hydraulic properties of a soil and different soils have different values of d (also see McBride and Horton, 1985). For a given d, n is proportional to S (also see Fig. 4). An overestimation of S will lead to an overestimation of n and thus an overestimation of α. The accuracy of estimating both α and n depends mainly on the accuracy of sorptivity estimation for a given soil because the determination of K_s, θ_s, θ_r, and θ_i should not produce large errors. Sorptivity estimation by fitting equation (24) to observed infiltration values is straight forward and hopefully does not allow for a large error either. Therefore this new infiltration method for estimating soil hydraulic properties should be accurate.

Conclusion

The integral method has been used to develop closed form approximate solutions to the problem of horizontal absorption. Solutions are used to estimate the parameters of hydraulic property models of Mualem (1976) and van Genuchten (1980). With a horizontal absorption experiment, saturated hydraulic conductivity is the only parameter needed to give complete information on hydraulic properties of a soil. The parameters, α and n, in the van Genuchten model (1980) are related for a given soil. The curve index, n, is estimated by the length of wetted zone and the sorptivity that can be measured in the horizontal absorption procedure. The scaling parameter, α, is estimated by saturated hydraulic conductivity, the length of wetted zone, and sorptivity. The approximate solutions presented here show in theory how to evaluate soil water characteristic curves and unsaturated hydraulic conductivity from simple horizontal infiltration experiments. Applications of this method may lead to saving time and expense in determining soil hydraulic properties.

References

Arya, L. M., and T. S. Dierolf. 1992. Predicting soil moisture characteristics from particle size distributions: An improved method to calculate pore radii from particle radii. p. 115-124. In M. Th. van Genuchten et al. (ed.) Proc. Int. Workshop on Indirect Methods for Estimating the Hydraulic Properties of Unsaturated Soils. Univ. of California, Riverside, California.

Brooks, R. H., and A. T. Corey. 1964. Hydraulic properties of porous media. Hydrol. Pap. 3. Colo. State Univ., Fort Collins, Colorado.

Brooks, R. H., and A. T. Corey. 1966. Properties of porous media affecting fluid flow. J. Irrig. Drain. Div. 92(IR2): 61-88.

Bruce, R. R., and A. Klute. 1956. The measurement of soil moisture diffusivity. Soil Sci. Soc. Am. Proc. 20: 458-462.

Clothier, B.E., and D.R. Scotter. 1982. Constant-flux infiltration from a hemispherical cavity. Soil Sci. Soc. Am. J. 46: 696-700.

Clothier, B.E., D.R. Scotter, and A. E. Green. 1983. Diffusivity and one-dimensional absorption experiments. Soil Sci. Soc. Am. J. 47: 641-644.

Dane, J. H., and W. E. Puckett. 1992. Field soil hydraulic properties based on physical and mineralogical information. p. 389-403. In M. Th. van Genuchten et al. (ed.) Proc. Int. Workshop on Indirect Methods for Estimating the Hydraulic

Properties of Unsaturated Soils. Univ. of California, Riverside, California.

Green, R.E., L.R. Ahuja, and S.K. Chong. 1986. Hydraulic conductivity, diffusivity, and sorptivity of unsaturated soils: Field methods. p. 771-798. In A. Klute (ed.) Methods of Soil Analysis. Part 1: Physical and Mineralogical Methods. Agronomy Monograph no. 9 (2nd edition). Soc. Agron. Am. and Soil Sci. Soc. Am. Madison, Wisconsin.

Jackson, R. D. 1963. Porosity and soil-water diffusivity relations. Soil Sci. Soc. Am. Proc. 27: 123-126.

Klute, A., and C. Dirksen. 1986. Hydraulic conductivity and diffusivity: Laboratory methods. p. 687-734. In A. Klute (ed.) Methods of Soil Analysis. Part 1: Physical and Mineralogical Methods. Agronomy Monograph no. 9 (2nd edition). Soc. Agron. Am. and Soil Sci. Soc. Am. Madison, Wisconsin.

Kool, J.B., J.C. Parker. 1988. Analysis of the inverse problem for transient unsaturated flow. Water Resour. Res. 24: 817-830.

Kool, J.B., J.C. Parker, and M. Th. van Genuchten. 1987. Parameter estimation for unsaturated flow and transport models-A review. J. Hydrol. 91: 225-293.

Landahl, H.D. 1953. An approximation method for the solution of diffusion and related problems. Bull. Math. Biophys. 15: 49-61.

McBride, J.F., and R. Horton. 1985. An empirical function to describe measured water distributions from horizontal infiltration experiments. Water Resour. Res. 21: 1539-1544.

Mualem, Y. 1976. A new model for predicting the hydraulic conductivity of unsaturated porous media. Water Resour. Res. 12: 593-622.

Neuman, S.P. 1973. Calibration of distributed parameter groundwater flow models viewed as a multiple-objective decision process under uncertainty. Water Resour. Res. 9: 1006-1021.

Nofziger, D. L. 1978. Errors in gamma-ray measurements of water content and bulk density in nonuniform soils. Soil Sci. Soc. Am. J. 42: 845-850.

Philip, J.R. 1957. The theory of infiltration, 6, Effect of water depth over soil. Soil Sci. 85: 278-286.

Philip, J.R. 1960. General method of exact solution of the concentration-dependent diffusion equation. Aust. J. Phys. 13: 1-12.

Prasad, S.N., and M.J.M. Romkens. 1982. An approximate integral solution of vertical infiltration under changing boundary conditions. Water Resour. Res. 18: 1022-1028.

Puckett, W. E., J. H. Dane, and B. F. Hajek. 1985. Physical and mineralogical data to determine soil hydraulic properties. Soil Sci. Soc. Am. J. 49: 831-836.

Reichardt, K., D. R. Nielsen, and J. W. Biggar. 1972. Scaling of horizontal infiltration into homogeneous soils. Soil Sci. Soc. Am. Proc. 36: 241-245.

Russo, D., E. Bresler, U. Shani, and J.C. Parker. 1991. Analyses of infiltration events in relation to determining soil hydraulic properties by inverse methodology. Water Resour. Res. 27: 1361-1373.

Selim, H. M., D. Kirkham, and M. Amemiya. 1970. A comparison of two methods for determining soil-water diffusivity. Soil Sci. Soc. Am. Proc. 34: 14-18.

Sisson, J. B., and M. Th. van Genuchten. 1991. An improved analysis of gravity drainage experiments for estimating the unsaturated hydraulic functions. Water Resour. Res. 27: 569-575.

Tyler, S. W., and S. W. Wheatcraft. 1989. Application of fractal mathematics to soil water retention estimation. Soil Sci. Soc. Am. J. 53: 987-996.

Tyler, S. W., and S. W. Wheatcraft. 1990. Fractal processes in soil water retention. Water Resour. Res. 26: 1047-1054.

van Genuchten, M. Th. 1992. On estimating the hydraulic properties of unsaturated soils. p. 1-14. In M. Th. van Genuchten et al. (ed.) Proc. Int. Workshop on Indirect Methods for Estimating the Hydraulic Properties of Unsaturated Soils. Univ. of California, Riverside, California.

van Genuchten, M. Th. 1980. A closed form equation for predicting the hydraulic conductivity of unsaturated soils. Soil Sci. Soc. Am. J. 44: 892-898.

Whisler, F. D., A. Klute, and D. B. Peters. 1968. Soil-water diffusivity from horizontal infiltration. Soil Sci. Soc. Am.

Proc. 32: 6-11.

Wu, L., and J. A. Vomocil. 1992. Predicting the soil water characteristic from the aggregate size-distribution. p. 139-145. In M. Th. van Genuchten et al. (ed.) Proc. Int. Workshop on Indirect Methods for Estimating the Hydraulic Properties of Unsaturated Soils. Univ. of California, Riverside, California.

Zimmerman, R.W., and G.S. Bodvarsson. 1989. Integral method solution for diffusion into a spherical block. J. Hydrol. 111: 213-224.

Zimmerman, R.W., G.S. Bodvarsson, and E.M. Kwicklis. 1990. Absorption of water into porous blocks of various shapes and sizes. Water Resour. Res. 26: 2797-2806.

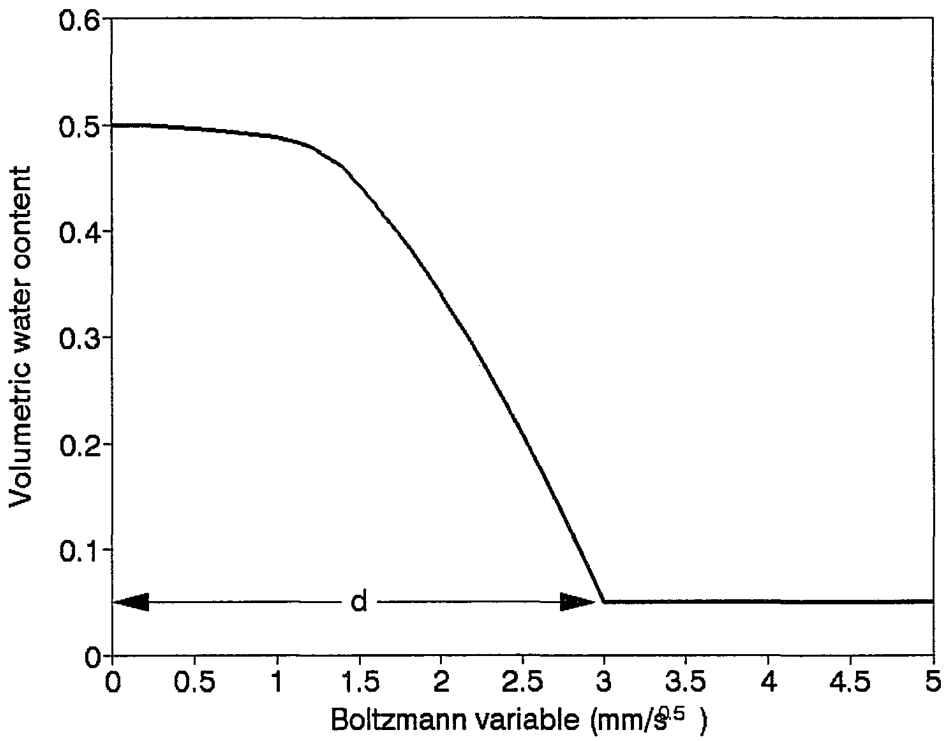

Figure 1. An assumed water content profile of horizontal infiltration.

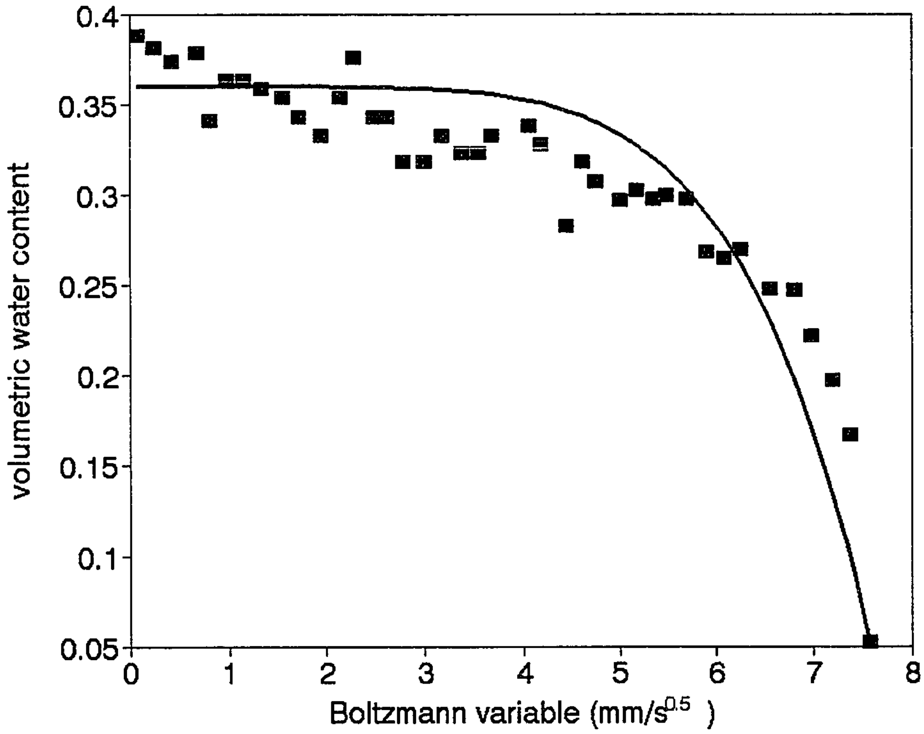

Figure 2a. Observed (filled square) and fitted (solid curve) soil water distribution data for Hagener sand.

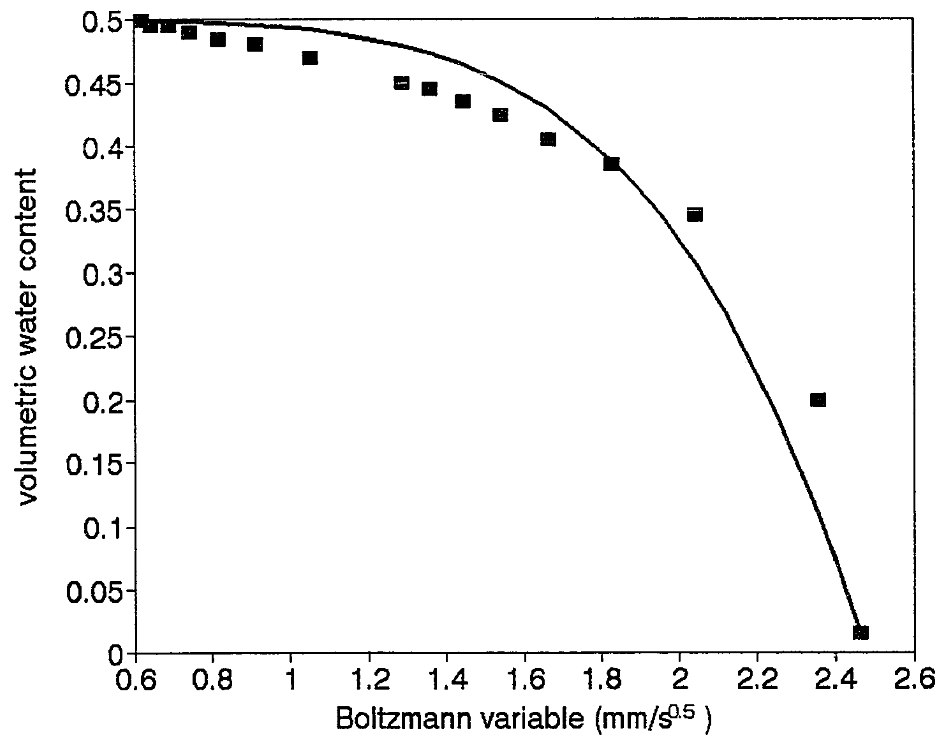

Figure 2b. Observed (filled square) and fitted (solid curve) soil water distribution data for Hayden sandy loam.

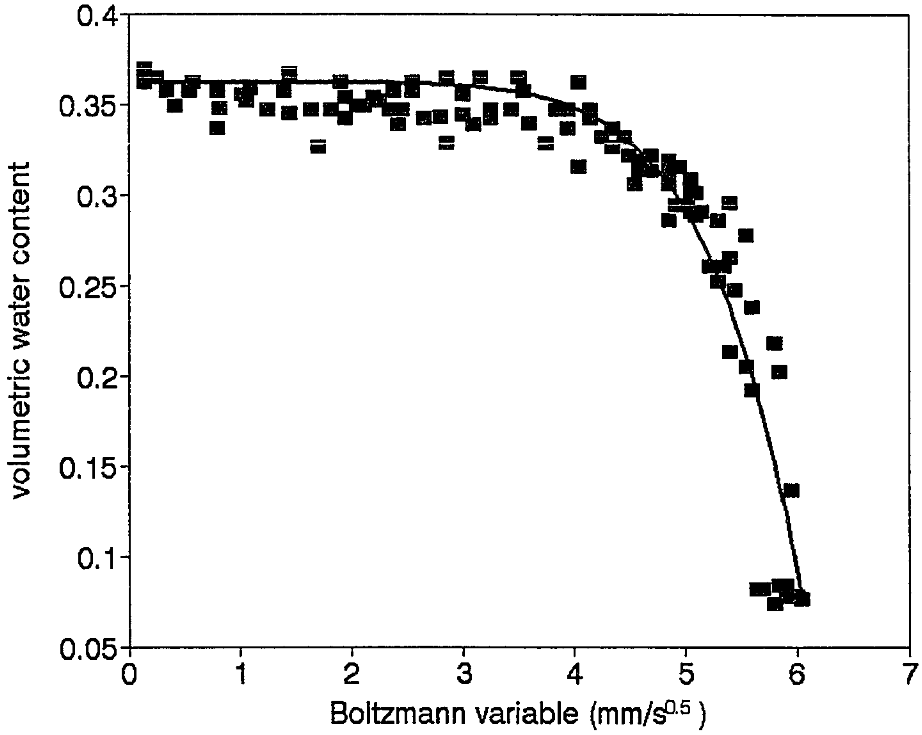

Figure 2c. Observed (filled square) and fitted (solid curve) soil water distribution data for Manawatu fine sandy loam.

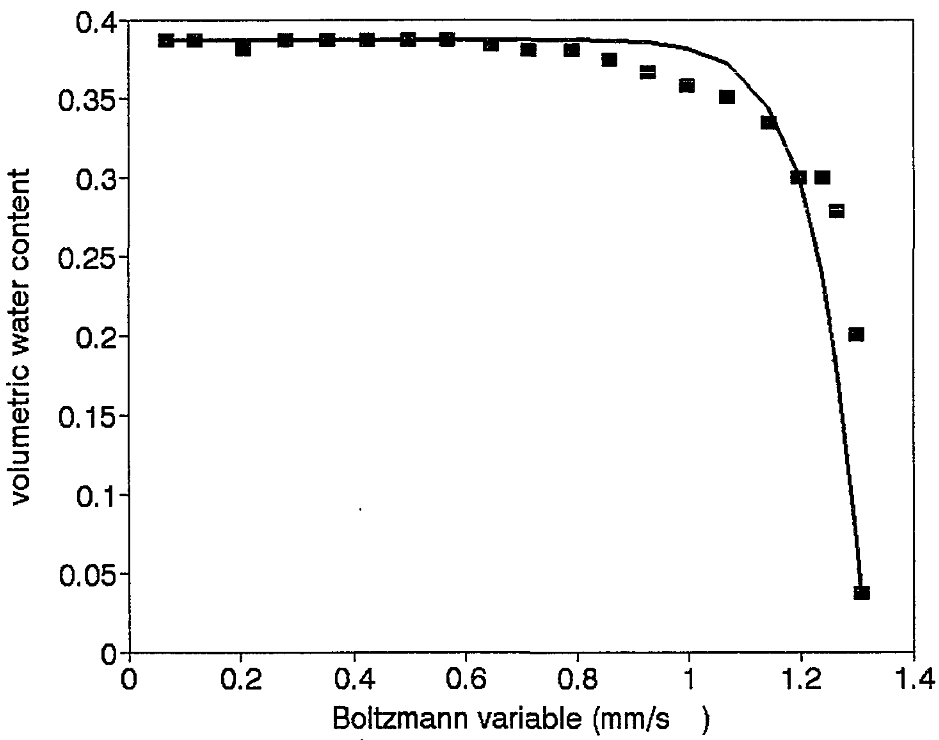

Figure 2d. Observed (filled square) and fitted (solid curve) soil water distribution data for Adelanto loam.

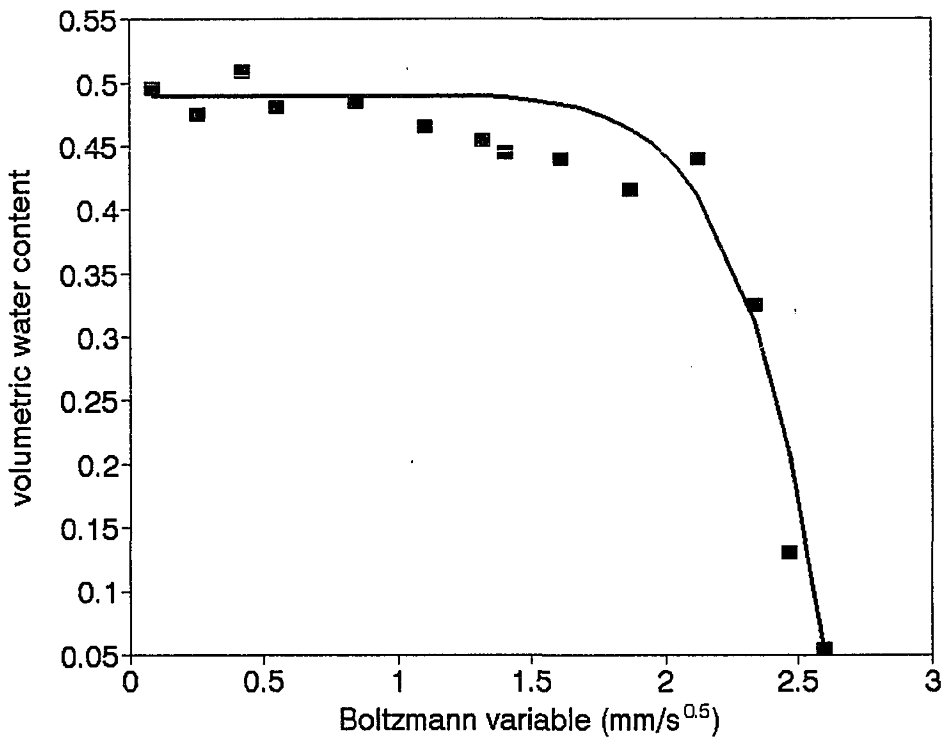

Figure 2e. Observed (filled square) and fitted (solid curve) soil water distribution data for Edina silt loam.

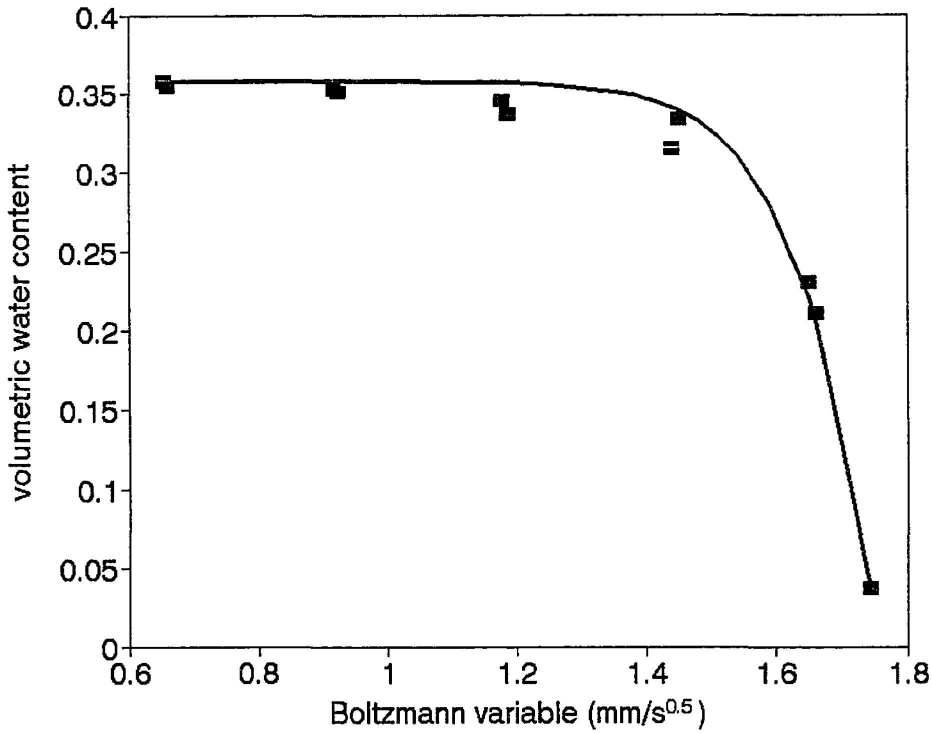

Figure 2f. Observed (filled square) and fitted (solid curve) soil water distribution data for Nicollet sandy clay loam.

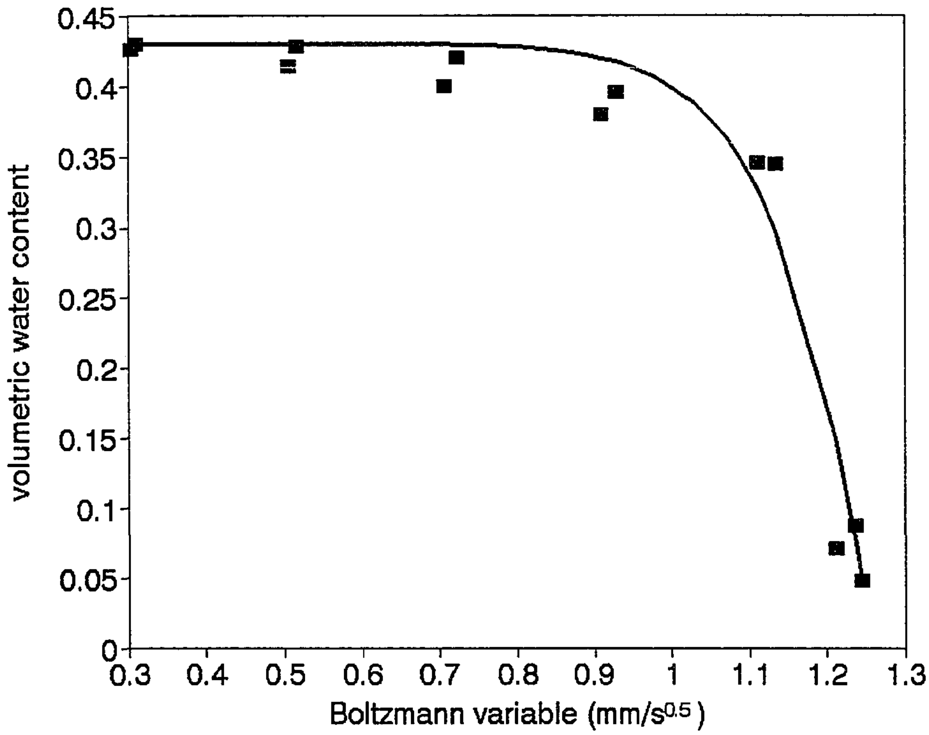

Figure 2g. Observed (filled square) and fitted (solid curve) soil water distribution data for Fayette silty clay loam.

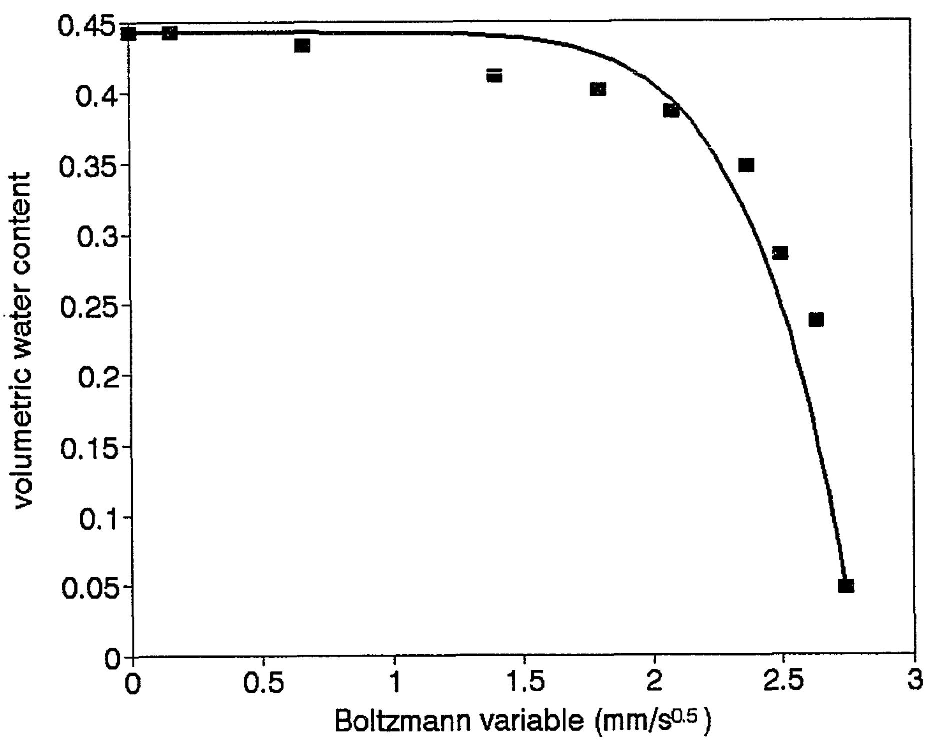

Figure 2h. Observed (filled square) and fitted (solid curve) soil water distribution data for Panoche clay loam.

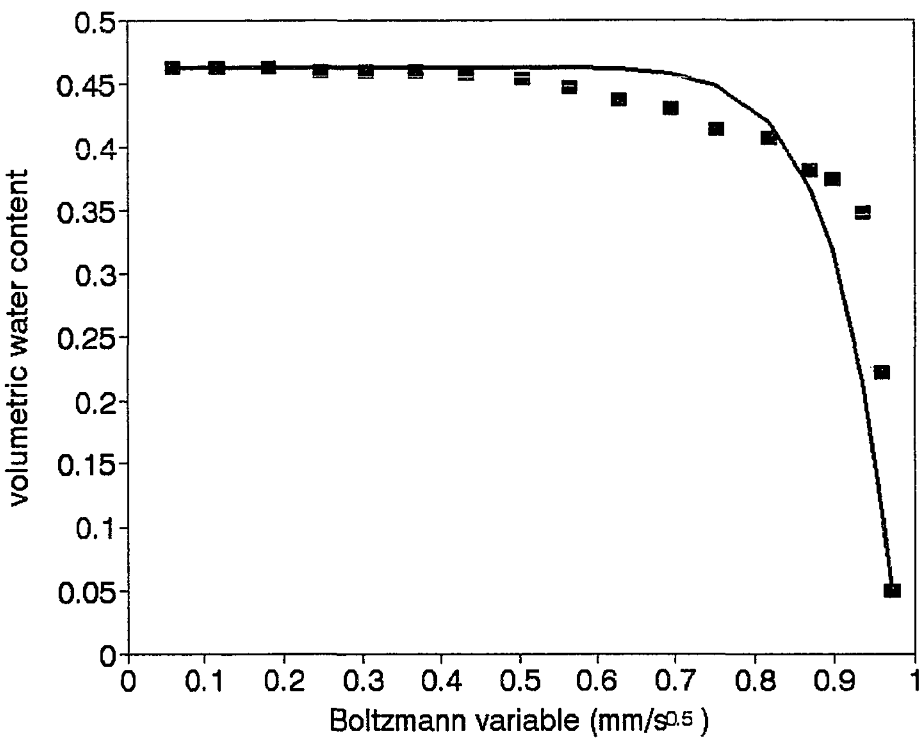

Figure 2i. Observed (filled square) and fitted (solid curve) soil water distribution data for Pine silty clay.

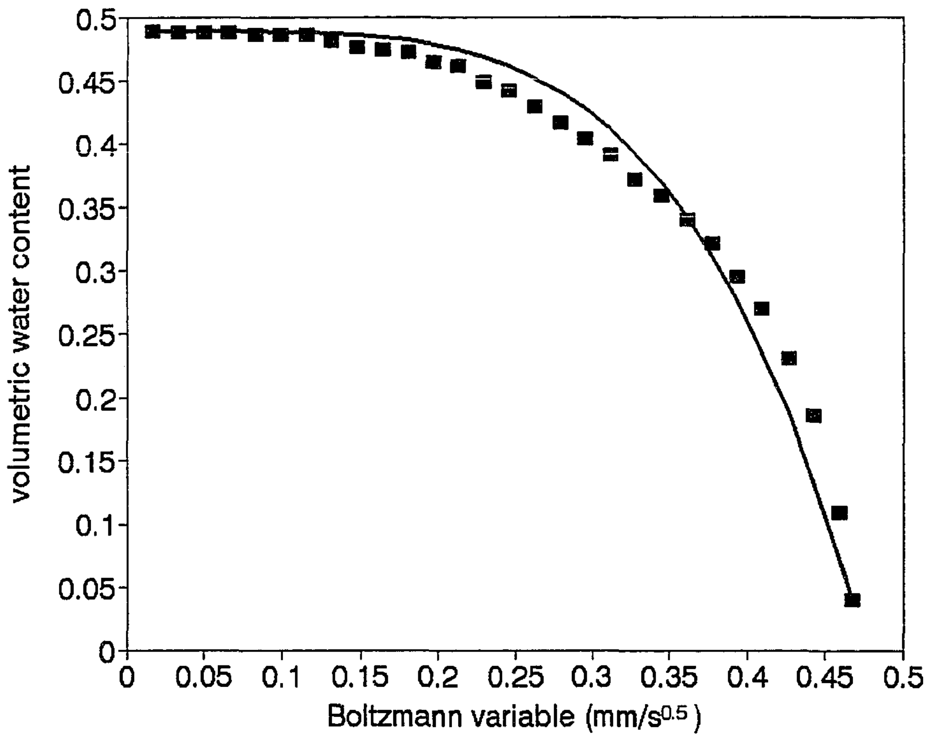

Figure 2j. Observed (filled square) and fitted (solid curve) soil water distribution data for Yolo clay.

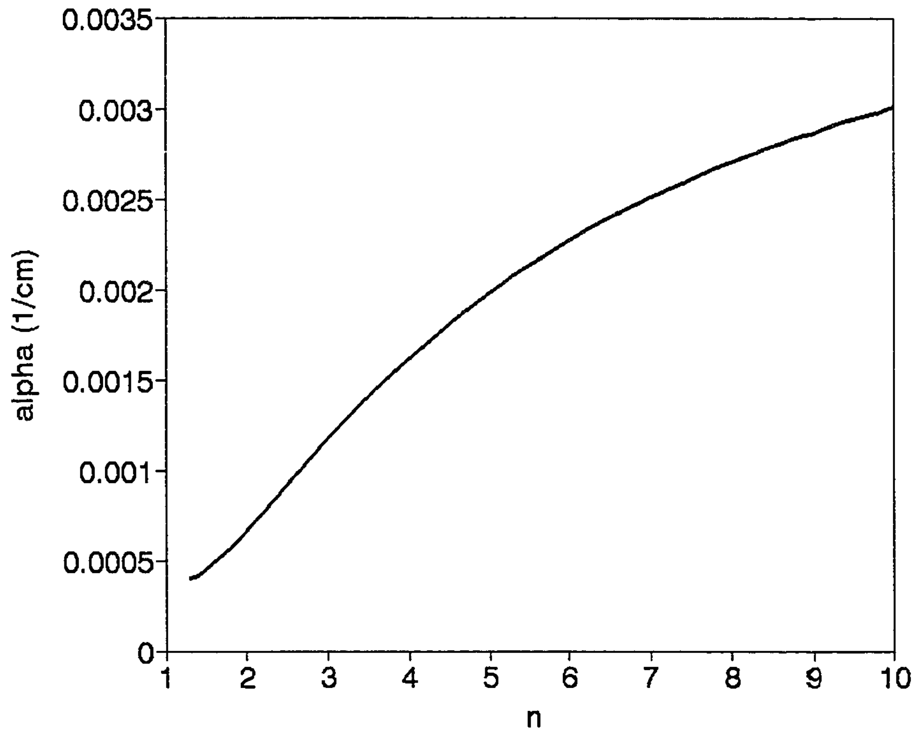

Figure 3. The relationship between scaling factor (α) and shape parameter (n) for a given soil.

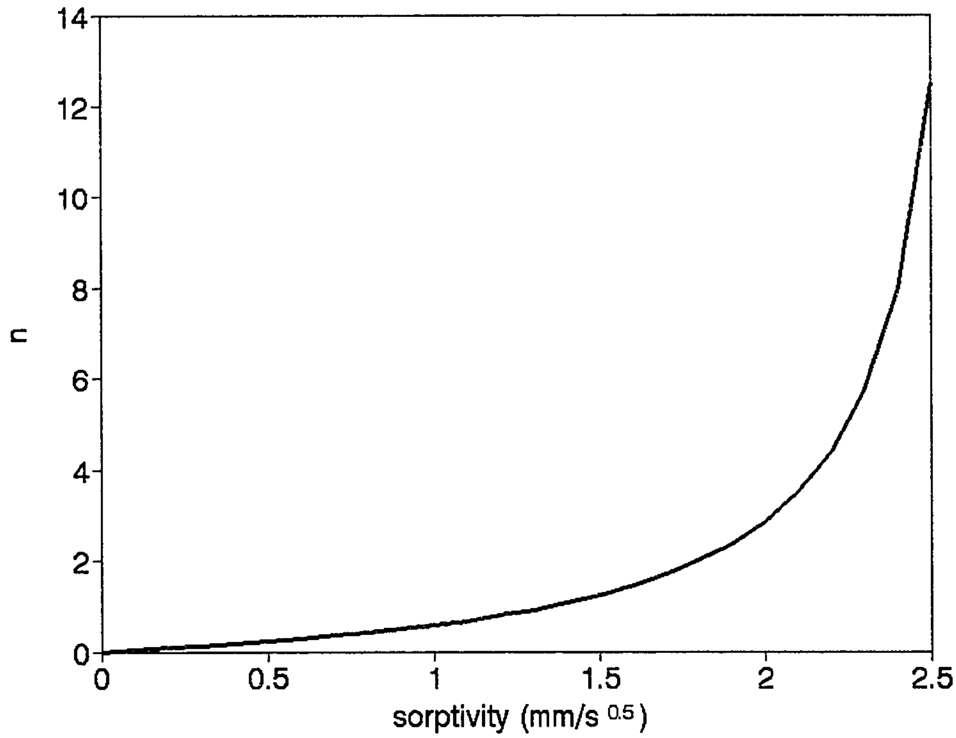

Figure 4. The relationship between shape parameter (n) and sorptivity (S) for a given soil.

CHAPTER 6. SIMPLE WATER INFILTRATION METHOD FOR ESTIMATING SOIL HYDRAULIC PROPERTIES: II. EXPERIMENTAL

A paper to be submitted to Soil Science Society of America Journal

Mingan Shao and Robert Horton

Abstract

To predict water flow, knowledge of soil hydraulic properties is required. Horizontal infiltration of water into soil columns can be observed in order to determine hydraulic properties. Required analysis of the observation is based on an integral solution of Richards' equation. The parameters of the characteristic curve are estimated by the observed length of wetted zone and sorptivity. Unsaturated hydraulic conductivity is estimated from the parameters determined in the soil characteristic curve and the measurement of saturated hydraulic conductivity. Six soils ranging from sandy loam to clay loam are included in this research. Soil characteristic curves for the six soils estimated by the infiltration method are in good agreement with measured characteristic curves. Unsaturated hydraulic conductivity, estimated by the infiltration method for the sandy loam, also compares well with measured values. The new method uses a transient approach to determine soil characteristic curves instead of

the usual equilibrium approach. The infiltration method provides a simple, accurate, and fast procedure for estimating soil hydraulic properties.

Introduction

Unsaturated water flow and chemical transport modeling usually requires the accurate and complete information about soil hydraulic properties. Soil hydraulic properties include a water characteristic curve (the relation between volumetric water content (θ) and pressure head (h)), θ(h); hydraulic conductivity (K); and water diffusivity (D). Because the three hydraulic properties are related by $K=D\ d\theta/dh$, only two of them are independent. Usually hydraulic conductivity and a water characteristic curve are considered to be two of the most important hydraulic properties. Unfortunately, the unsaturated hydraulic properties are very difficult to measure or estimate. Great effort has been made to measure or estimate soil hydraulic properties for several decades (e.g., Bruce and Klute, 1956; Rose et al., 1965; Dirksen, 1975; Green et al., 1986; Sisson and van Genuchten, 1991). Many laboratory and field methods have been proposed, and detailed reviews of the methods have been given by Green et al. (1986), Klute and Dirksen (1986), and van Genuchten (1992). Most methods lack accuracy, however, and are time consuming, need specialized and costly equipment, require special operating skill, or only provide data over a very limited range (Plagge et al., 1992; de Jong et al., 1992). Because of these limitations, estimations of soil hydraulic properties from an easy experiment or easily observed properties may have potential attraction to experimental soil physicists.

This paper presents a new and simple infiltration method, based essentially on the solution to Richards' equation of horizontal infiltration, that uses the closed-form functions of van Genuchten (1980) to describe soil hydraulic properties. This paper also presents comparisons of predicted and measured soil hydraulic properties. The theoretical analysis of the integral method was presented in Shao and Horton (1996). The equations for estimating the scaling parameter (α) and shape parameter (n) are

$$\alpha=\frac{2(n+1)K_s}{n(\theta_s-\theta_i)d^2}\left[\frac{1}{m}\left(\frac{\theta_s-\theta_i}{\theta_s-\theta_r}\right)\right]^{\frac{1}{n}} \tag{1}$$

$$n=\frac{S}{d(\theta_s-\theta_i)-S} \tag{2}$$

where θ_s is saturated water content; θ_r is the residual water content; K_s is the saturated hydraulic conductivity; S is sorptivity; θ_i is the initial water content; m=1-1/n; and d is the characteristic length of wetted zone. Equations (1) and (2), representing the parameter estimation of the van Genuchten model (1980) of soil hydraulic properties, include six parameters, K_s, S, d, θ_s, θ_r, and θ_i. The two water contents, θ_s and θ_i, are easy to measure; θ_r needs to be estimated (for example, taking the water content at -15 bar pressure potential as θ_r). S is also relatively easy to obtain. The characteristic length of wetted zone (d) can be observed easily. The last parameter is the saturated hydraulic conductivity that can be conveniently measured. With the parameters (α, n, and K_s), the soil characteristic curve and hydraulic conductivity can be predicted from the van Genuchten (1980) equations.

Materials and Methods

Six soils were used to test the integral approach in this study. The first five soils are a silt loam obtained from land mapped as the Flagler series(Coarse-loamy, mixed, mesic Typic Hapludoll, 0.114 sand, 0.700 silt, and 0.186 clay mass fractions), Nicollet loam (Fine-loamy, mixed, mesic Aquic Hapludoll, 0.509 sand, 0.326 silt, and 0.165 clay), Keswick sandy clay loam (Fine, Montmorillontic, mesic Aquic Hapludoll, 0.677 sand, 0.113 silt, and 0.210 clay), Monona silty clay loam (Fine-silty, mixed, mesic Typic Hapludoll, 0.024 sand, 0.695 silt, and 0.281 clay), and Webster clay loam (Fine-loamy, mixed, mesic, Typic Endoaquoll, 0.321 sand, 0.392 silt, and 0.287 clay). The sixth soil is Manawatu fine sandy loam (a Dystric Fluventic Eutrochrept). Information on the hydraulic properties of the sixth soil was obtained from

Clothier and Scotter (1982).

Some basic physical properties of the first five soils were measured. The specific surface areas were measured by using the EGME technique (Chihacek and Bremner, 1979; Carter et al., 1986). Particle densities were determined by using the pycnometer method (Blake and Hartge, 1986a). Bulk densities were also determined by the clod method (Blake and Hartge, 1986b). The saturated water contents of the five soils were obtained by measuring both mass water contents and their bulk densities at saturation. The residual water contents were estimated as the water contents at -15 bar pressure potential (van Genuchten, 1980).

The soil characteristic curves for the first five soils were measured by the pressure plate technique. Additionally, traditional horizontal-infiltration experiments of the Bruce-Klute type (1956) were performed. Air-dried soil was packed into sectioned plexiglas tubes 0.15 m long (15 sections) and 0.038 m in diameter with the controlled bulk density of 1.30 Mg/m^3. During infiltration, water was supplied to one end of the soil column by a burette through a ceramic plate. During the horizontal infiltration (absorption), the advance of the wetting front with time and the amount of water infiltrated into the soil column were recorded. The horizontal absorption experiment was ended when the wetting front reached about half the length of the column. The saturated hydraulic conductivities of the first five soils were measured by a constant head technique (Klute and Dirksen, 1986).

Results and Discussion

The particle densities (ρ_s) and specific surfaces (SS) of the first five soils, together with saturated water contents (θ_s) and residual water contents (θ_r) of all six soils are listed in Table 1.

Table 1. Some physical properties of the five soils

soil	SS	ρ_s	θ_s	θ_r
	(10^{-3} m^2/kg)	(Mg/m^3)	(m^3/m^3)	(m^3/m^3)
sandy loam	—	—	0.440	0.000
silt loam	41	2.67	0.502	0.118
loam	40	2.69	0.503	0.130
sandy clay loam	58	2.64	0.542	0.115
silty clay loam	79	2.67	0.562	0.163
clay loam	141	2.57	0.569	0.182

The saturated water content for fine sandy loam was obtained by averaging the first three measured water contents near saturation from the data of Clothier and Scotter (1982, Fig. 1 in their paper) because the water content near saturation seemed to be irregular. The residual water content was assumed to be zero for the fine sandy loam. This assumption may be safe for such a coarse textured soil, and by using the van Genuchten model (1980), the regression results of the water characteristic curve also gave a zero residual water content.

The three important parameters for estimating α and n are sorptivity (S), saturated hydraulic conductivity (K_s), and characteristic wetted length (d) (values of the Boltzmann variable at wetting fronts). Here they are referred to as hydraulic parameters. The repeatability of these three parameters is important. Table 2 presents the parameters obtained from three separate infiltration experiments using sandy clay loam. The parameters have small variation and indicating good repeatability.

An example of calculating n and α may be helpful. For sandy clay loam (also see Table 2), the average value of S is found to be 6.47×10^{-4} $m/s^{1/2}$. The S values are obtained by

Table 2. The hydraulic parameters for sandy clay loam

column	S	K_s	d
	(10^{-4} $m/s^{1/2}$)	(10^{-7} m/s)	(10^{-3} $m/s^{1/2}$)
1	6.34	5.26	1.96
2	6.06	4.89	1.86
3	7.02	5.74	2.17
mean	6.47	5.30	2.00

curve-fitting (Shao and Horton, 1996 equation (24)) the observed infiltration data; the mean of d is 1.96×10^{-3} m/s$^{1/2}$ (the value of the Boltzmann variable obtained from the wetting front at the end of the infiltration experiment); the average value of K_s is 5.30×10^{-7} m/s (measured by the constant head technique (Klute and Dirksen, 1986)); the values of θ_s, θ_r, and θ_i are 0.54, 0.12, and 0.002, respectively; using equation (2) in this paper and the above values of d, S, θ_s, and θ_i n is found to be 1.59; using equation (1) in this paper and the above values of K_s, d, θ_s, θ_r, and θ_i α is found to be 1.51 m^{-1}.

The values of the hydraulic parameters for the six soils are shown in Table 3. The parameters of the sandy loam were taken from the literature (Clothier and Scotter, 1982; Clothier and Wooding, 1983). The saturated hydraulic conductivity of silty clay loam is smaller than that of clay loam. This can be explained in part by the particle compositions. The silty clay loam has almost the same clay content (.281) as that of clay loam (.287), but the silty clay loam contains much less sand (0.024) than the clay loam (0.321). Table 3 shows that both sorptivity and the characteristic wetting length tend to decrease when soils become finer in texture. With measured values of the parameters, K_s, S, d, θ_s, θ_i, and estimated θ_r, parameters α and n can be determined from Eqs. (1) and (2).

Table 3. The hydraulic parameter values for six soils

soil	S (10^{-4} m/s$^{1/2}$)	K_s (10^{-7} m/s)	d (10^{-3} m/s$^{1/2}$)
sandy loam	14.70	201.00	6.05
silt loam	9.87	20.17	3.50
loam	9.84	17.80	3.44
sandy clay loam	6.47	5.30	2.00
silty clay loam	6.03	1.11	1.70
clay loam	5.16	3.36	1.55

The calculated values of α and n from the integral method for all six soils, together with those determined by curve-fitting the actual water characteristic curve data with the van Genuchten model (1980), are listed in Table 4. The measured saturated water content (θ_s) and estimated residual water content (θ_r) and those obtained by curve-fitting are also included in Table 4. The α values and n values from both the infiltration method and from curve-fitting (van Genuchten, 1980) show similar treads of decreasing from sandy loam (coarser texture) to clay loam (finer texture). In general curve-fit values of θ_s and θ_r are consistently lower than the values of θ_s and θ_r observed for each soil. The fitted residual water contents do not have a clear relationship to soil textures.

Table 4. The parameter values for six soils

soil	Infiltration Method				Curve Fitting			
	α	n	θ_s	θ_r	α	n	θ_s	θ_r
sandy loam	2.65	3.15	0.44	0.00	2.63	3.05	0.43	0.00
silt loam	4.97	1.45	0.50	0.12	10.23	1.18	0.50	0.00
loam	5.13	1.43	0.50	0.13	16.81	1.16	0.50	0.00
sandy clay loam	1.51	1.59	0.54	0.12	0.35	1.94	0.51	0.12
silty clay loam	0.51	1.79	0.56	0.16	0.59	1.14	0.53	0.10
clay loam	1.12	1.71	0.56	0.18	1.23	1.38	0.54	0.13

The soil characteristic curves of the first five soils estimated from the infiltration method are compared with those measured by pressure plate technique (from Figure 1b to Figure 1f). Comparison data (Figure 1a)for the sixth soil (sandy loam) is taken from the literature (Clothier and Scotter, 1982). The fitted characteristic curves for all six soils, obtained by fitting the closed form equation of van Genuchten (1980) to the observed data, are also shown in Figure 1 (Fig. 1a - Fig. 1f). Generally, the soil characteristic curves estimated by the infiltration method are in good agreement with the observed data for all six soils. The estimated characteristic curves for the first five soils tend to overestimate water contents in the range of 0 to -1 m in pressure potential and underestimate water contents for the range of -1 to -10 m in pressure potential. When pressure potential is less than -10 m the estimated characteristic curves compare well with the measured ones. The estimated curves indicate greater water contents than the fitted curves near saturation because the measured saturated water contents are consistently larger than those determined by curve-fitting. The estimated curves cross with the fitted curves somewhere near the -1 m pressure potential.

Hydraulic conductivities estimated by α and n values obtained from the infiltration method and from curve-fitting (Mualem, 1976; van Genuchten, 1980) are compared with the measured hydraulic conductivity of the sandy loam soil (Figure 2). Hydraulic conductivities estimated from the infiltration method and from curve-fitting water characteristic data are almost the same as the measured ones when pressure potential is greater than -0.2 m. For lower pressure potential (less than -0.2m) both methods overestimate hydraulic conductivity.

Conclusions

The experimental evidence provided in this study shows that a simple infiltration method can be used to estimate soil hydraulic properties. The α and n parameters in the closed-form equation (van Genuchten, 1980), estimated by the infiltration method, show a relation with soil texture. The soil water characteristic curves estimated by the infiltration method are in good agreement with those observed for all six soils. Several weeks are needed to measure the water characteristic curves of six soils by using pressure plate equipment whereas this can be accomplished with the infiltration method in several days by using very simple equipment (horizontal infiltration device). The infiltration method can simultaneously estimate both soil characteristic curve and unsaturated hydraulic conductivity from one simple horizontal infiltration experiment. Therefore, the infiltration method does not need specialized and expensive equipment and does not require substantial special operation skills either. The new infiltration method provides an attractive approach for estimating soil hydraulic properties.

References

Blake, B. R., and K. H. Hartge. 1986a. Particle density. Method of Soil Analysis. ASA monograph no. 9: 377-382.

Blake, B. R., and K. H. Hartge. 1986b. Bulk density. Method of Soil Analysis. ASA monograph no. 9: 363-375.

Bruce, R. R., and A. Klute. 1956. The measurement of soil moisture diffusivity. Soil Sci. Soc. Am. Proc. 20: 458-462.

Carter, D.L., M.M. Mortland, and W.D. Kemper. 1986. Specific surface. Method of Soil Analysis, ASA monograph no. 9: 413-423.

Chihacek, L.J., and J.M. Bremner. 1979. A simplified ethylene glycol monoethyl ether procedure for assessment of soil surface area. Soil Sci. Soc. Am. J. 43: 821-822.

Clothier, B. E., and D. R. Scotter. 1982. Constant-flux infiltration from a hemispherical cavity. Soil Sci. Soc. Am. J. 46: 696-700.

Clothier, B. E., and R. A. Wooding. 1983. The soil water diffusivity near saturation. Soil Sci. Soc. Am. J. 47: 636-640.

de Jong, R., G.C. Topp, and W.D. Reynolds. 1992. The use of measured and estimated hydraulic properties in the simulation of soil water movement - A case study. p. 569-584. *In* M.Th. van Genuchten et al. (ed.) Proc. Int. Workshop on Indirect Methods for Estimating the Hydraulic Properties of Unsaturated Soils. Univ. of California, Riverside, California.

Dirksen, C. 1975. Determination of soil water diffusivity by sorptivity measurements. Soil Sci. Soc. Am. J. 39: 22-27.

Green, R.E., L.R. Ahuja, and S.K. Chong. 1986. Hydraulic conductivity, diffusivity, and sorptivity of unsaturated soils: Field methods. p. 771-798. *In* A. Klute (ed.) Methods of Soil Analysis, Part 1, Physical and Mineralogical Methods. Agronomy Monograph no. 9 (2nd edition). Soc. Agron. Am. and Soil Sci. Soc. Am. Madison, Wisconsin.

Klute, A., and C. Dirksen. 1986. Hydraulic conductivity and diffusivity: Laboratory methods. p. 687-734. *In* A. Klute (ed.) Methods of Soil Analysis, Part 1, Physical and Mineralogical Methods. Agronomy Monograph no. 9 (2nd edition). Soc. Agron. Am. and Soil Sci. Soc. Am. Madison, Wisconsin.

Mualem, Y. 1976. A new model for predicting the hydraulic conductivity of unsaturated porous media. Water Resour. Res. 12: 593-622.

Plagge, R., C.H. Roth, and M. Renger. 1992. A new laboratory method to rapidly determine the unsaturated soil hydraulic properties. p. 653-663. *In* M.Th. van Genuchten et al. (ed.) Proc. Int. Workshop on Indirect Methods for Estimating the Hydraulic Properties of Unsaturated Soils. Univ. of California, Riverside, California.

Rose, C. W.,W.R. Stern, and J.E. Drummond. 1965. Determination of hydraulic conductivity as a function of depth and water content for soil in situ. Water Resour. Res. 3: 1-9.

Sisson, J.B., and M. Th. van Genuchten. 1991. An improved analysis of gravity drainage experiments for estimating the unsaturated hydraulic functions. Water Resour. Res. 27: 569-575.

van Genuchten, M. Th. 1992. On estimating the hydraulic properties of unsaturated soils. p. 1-14. *In* M.Th. van Genuchten et al. (ed.) Proc. Int. Workshop on Indirect Methods for Estimating the Hydraulic Properties of

Unsaturated Soils. Univ. of California, Riverside, California.

van Genuchten, M. Th. 1980. A closed form equation for predicting the hydraulic conductivity of unsaturated soils. Soil Sci. Soc. Am. J. 44: 892-898.

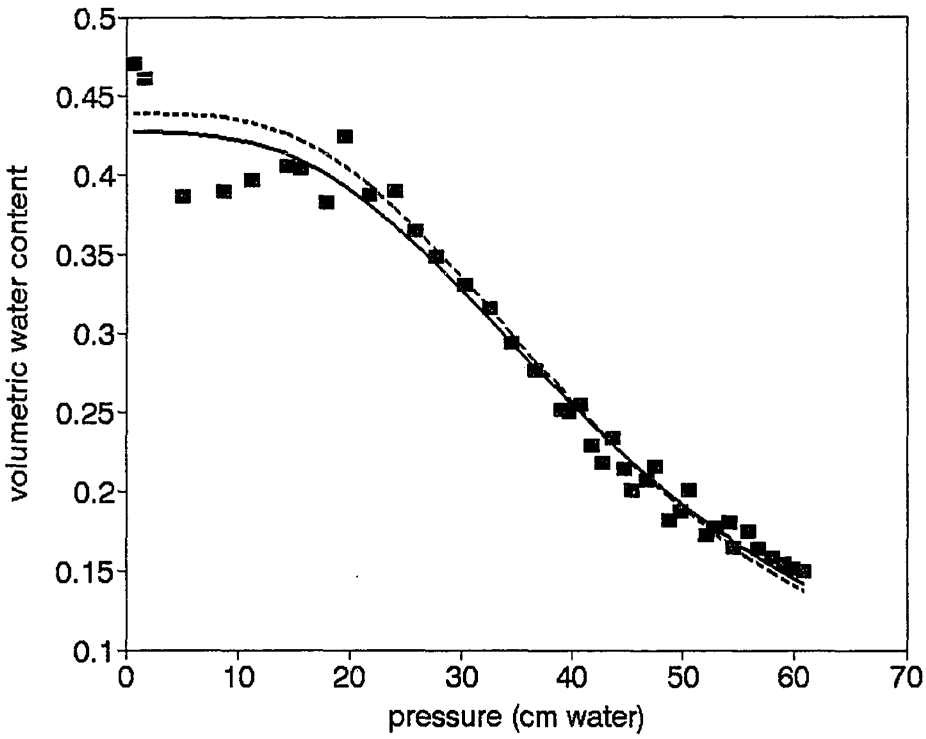

Figure 1a. Comparison of water characteristic curves obtained by the infiltration method (dashed curve) and by curve-fitting (solid curve) with observed data (filled square) for fine sandy loam.

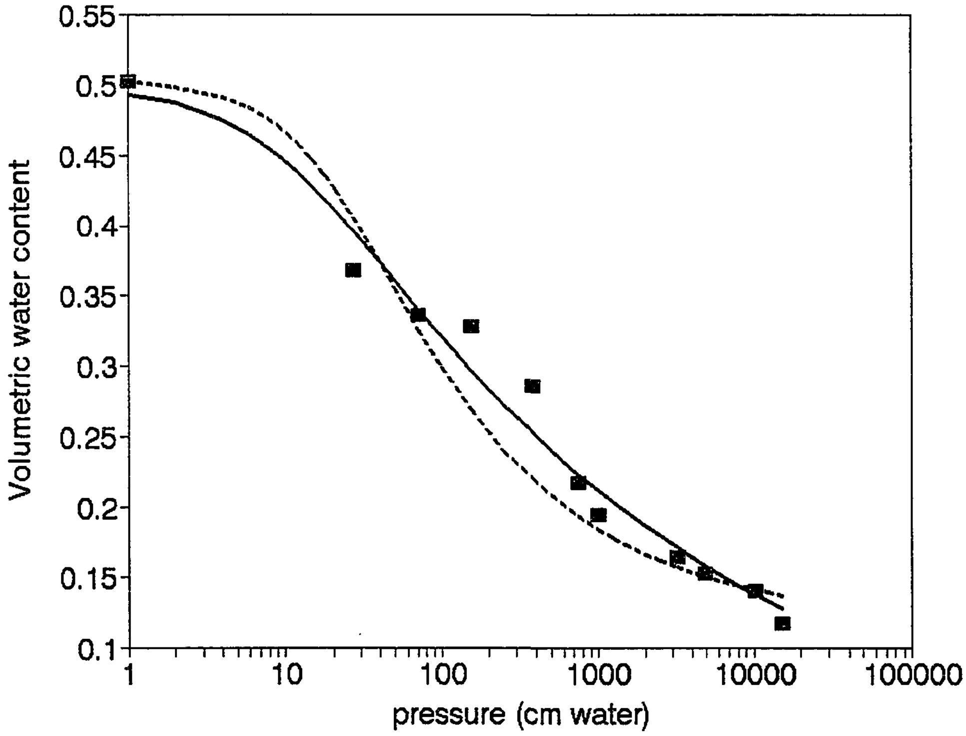

Figure 1b. Comparison of water characteristic curves obtained by the infiltration method (dashed curve) and by curve-fitting (solid curve) with observed data (filled square) for silt loam.

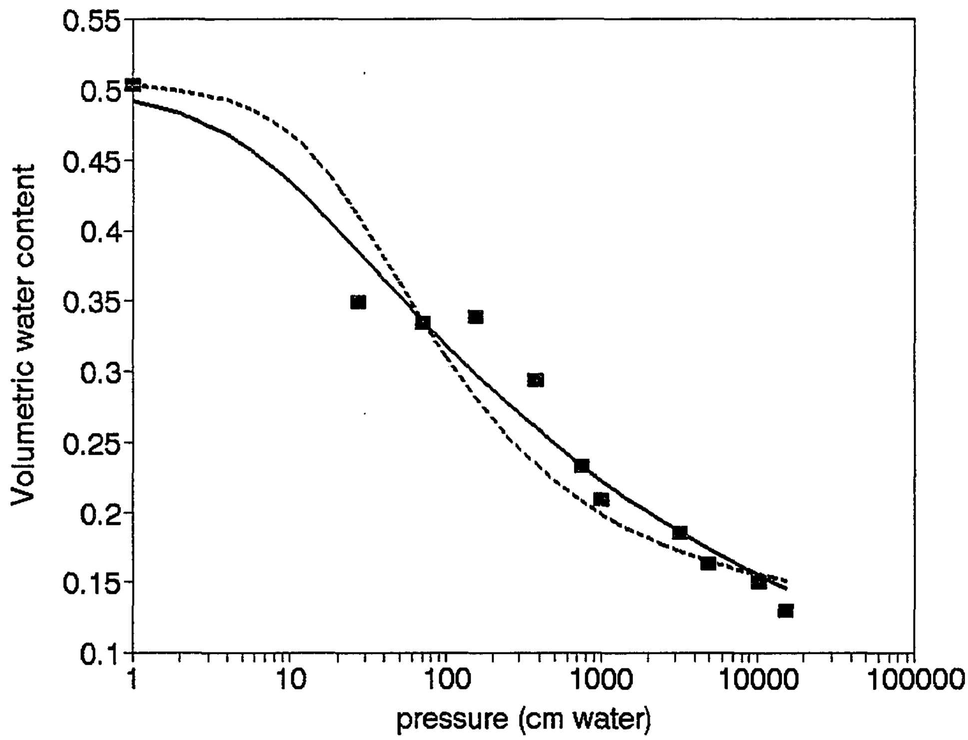

Figure 1c. Comparison of water characteristic curves obtained by the infiltration method (dashed curve) and by curve-fitting (solid curve) with observed data (filled square) for loam.

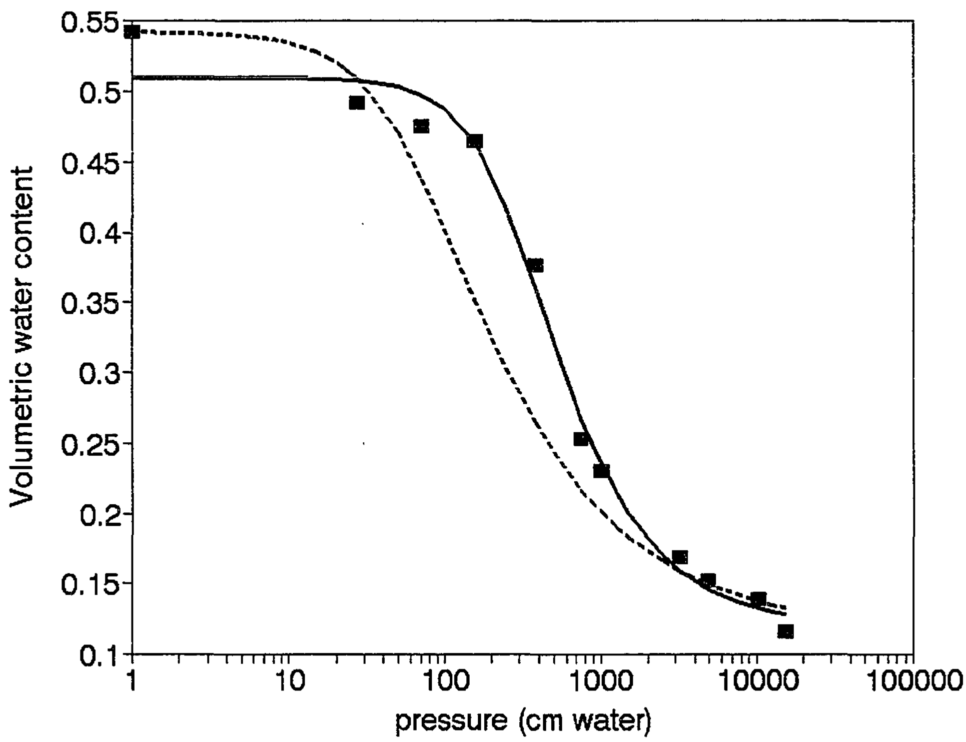

Figure 1d. Comparison of water characteristic curves obtained by the infiltration method (dashed curve) and by curve-fitting (solid curve) with observed data (filled square) for sandy clay loam.

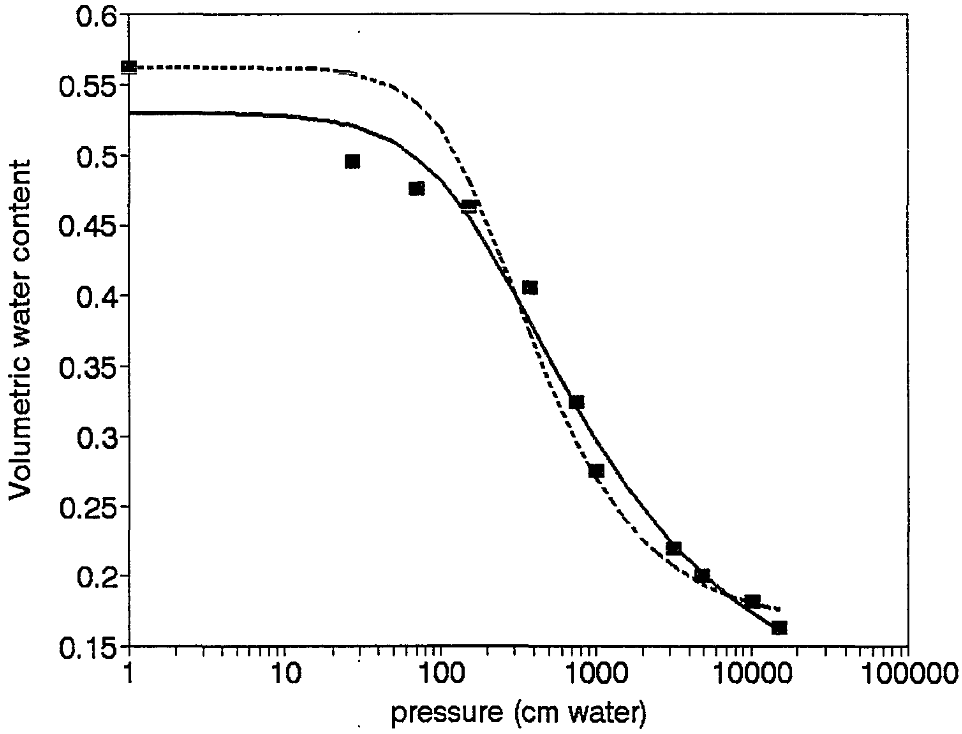

Figure 1e. Comparison of water characteristic curves obtained by the infiltration method (dashed curve) and by curve-fitting (solid curve) with observed data (filled square) for silty clay loam.

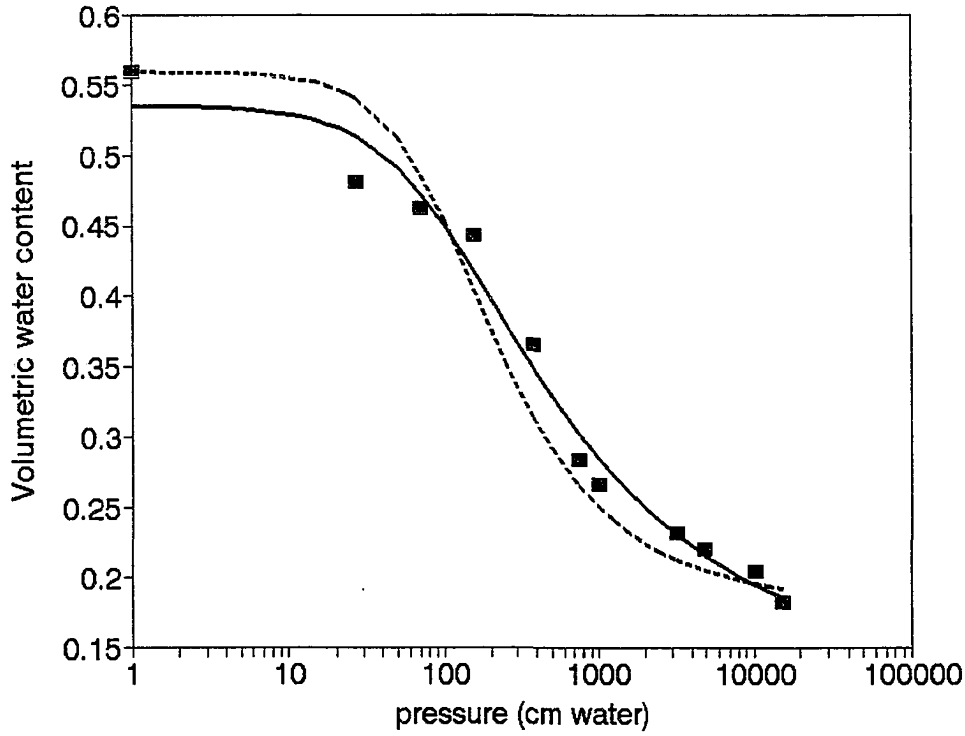

Figure 1f. Comparison of water characteristic curves obtained by the infiltration method (dashed curve) and by curve-fitting (solid curve) with observed data (filled square) for clay loam.

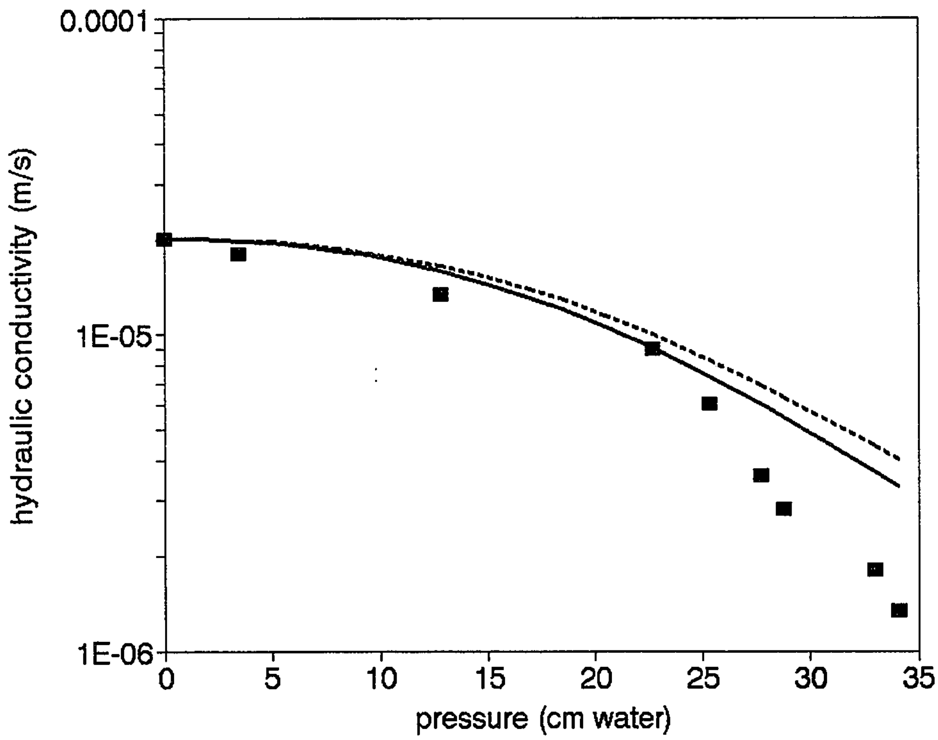

Figure 2. Comparison of unsaturated hydraulic conductivities obtained by the infiltration method (dashed curve) and by curve-fitting (solid curve) with observed data (filled square) for fine sandy loam.

CHAPTER 7. ESTIMATION OF SOLUTE TRANSPORT PARAMETERS BY BOUNDARY LAYER THEORY

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Abstract

This paper uses a boundary layer method to solve the convection-dispersion equation (CDE) in order to predict solute transport in soil. The boundary layer solution describing chemical transport for a semi-infinite soil column or field soil profile holds advantage of simplicity in expression and flexibility in manipulation over the corresponding exact solution to the CDE. Comparisons of the boundary layer solution to the exact solution are conducted for a range of parameter values. Results show that the boundary layer solution is in good agreement with the exact solution. An important manipulation of the boundary layer solution is to estimate transport parameters of solute movement through soils both under laboratory and field conditions. This leads to a new method for estimating parameters of solute transport in soils. The new method requires observation of the advance of the depth of boundary layer (solute front) with time. This can be done visually by

using a tracer solution with dye in it. The new method provides simplicity, saves time, and is applicable to both laboratory soil columns and field soils.

Introduction

Transport phenomena of agrichemicals through soils are significant processes in both crop production and groundwater quality control. Concern about the transport behavior of various chemicals in soils has resulted in the development of a number of theoretical models describing the basic mechanisms of chemical transport in soils (Parker and van Genuchten, 1984). With the development of more and more sophisticated models, increasing effort has been focused on estimating various model parameters for several decades (e.g. Rifai et al., 1956; Elprince and Day, 1977; Kool et al., 1987; Buchter et al., 1995). Two most common transport parameters are dispersion coefficient and retardation factor because most models of solute transport contain these two parameters.

The methods of estimating transport parameters are divided into statistical methods and deterministic methods. Statistical parameter estimation techniques, such as least-squares methods, maximum-likehood procedures, and method of moments, have proven to be useful (e.g. Elprince and Day, 1977; Parker and van Genuchten, 1984; Jury and Sposito, 1985; Bresler and Naor, 1987). However, some problems, such as parameter uncertainty and uniqueness, are still unsolved in statistical methods. Moreover, in practice there is a time assignment bias in estimating transport parameters by curve-fitting (least-squares method) transport models to breakthrough curve data (Schnabel and Richie, 1987). On the other hand, deterministic methods have advantages of clear concept and uniqueness of parameter estimation. However, the current deterministic methods can only be used to some limited cases of solute transport. For example, the method presented by Rifai et al. (1956) can only be used to estimate dispersion coefficient of convection-dispersion equation (CDE) for a first-type (concentration-type) inlet boundary condition. But the most appropriate inlet boundary for most or all solute displacement experiments is a third-type (flux-type) condition. (van Genuchten and Parker, 1984; 1994) instead of a first-type inlet boundary condition. The Rifai et al. (1956) method is exact but difficult to apply in practice because of limited use of breakthrough data (Yamaguchi et al., 1989). Though Rifai et al. (1956) method is modified by Yamaguchi et al. (1989) by using additional solute breakthrough data, but is still restricted to the first-type inlet boundary condition for estimating transport parameters of CDE.

In this paper a new method is proposed to estimate both dispersion coefficient and retardation factor simultaneously by using boundary layer theory. Boundary layer theory, an integral method, has been used previously to solve heat and mass transfer problems (e.g., Kumar and Narang, 1967; Gupta, 1974). In this present application of boundary layer theory to solute transfer problems for semi-infinite columns it is assumed that a chemical boundary layer analogous to the thermal boundary layer in heat transfer and to the velocity boundary layer in mass transfer exists whose thickness increases with time. The thickness of the boundary layer is specified by the distance from the surface down to the interface where conditions of zero solute flux and equality of resident concentration to its initial value are satisfied (depth of solute front). The solute front as a function of time can be used to determine dispersion coefficient and retardation factor.

Theory

One-dimensional transient solute transport through a homogeneous medium during steady-water flow is traditionally described by the following partial differential equation (CDE)

$$R\frac{\partial C_r}{\partial t} = D\frac{\partial^2 C_r}{\partial x^2} - v\frac{\partial C_r}{\partial x} \qquad \textbf{(1)}$$

where C_r is the volume-average (resident) solution concentration, D is the dispersion coefficient, v is the average pore-water velocity, R is the retardation factor, x is position, and t is time.

The initial condition for a displacement experiment semi-infinite space is

$$C_r(x,0)=0 \tag{2}$$

Equation (2) represents a soil column that is initially free of any solute. However, our analysis is easily extended to the case of a uniform initial concentration (C_i) by a simple variable substitution, i.e. $C_r'=C_r-C_i$. The most appropriate boundary conditions for solute displacement experiments (van Genuchten and Parker, 1984; 1994) are

$$\left(-D\frac{\partial C_r}{\partial x}+vC_r\right)\Big|_{x=0^+}=vC_0 \tag{3}$$

$$\left(\frac{\partial C_r}{\partial x}\right)\Big|_{x\to\infty}=0 \tag{4}$$

Equation (3) is valid for a system in which the entrance reservoir is not physically connected to the column and for systems where the column is connected directly to the entrance reservoir as long as diffusion across the inlet boundary is small relative to convective transport by water flow (van Genuchten and Parker, 1984; 1994).

It is assumed that there is a boundary layer (see Fig. 1), d(t), where d(t) is the depth of the solute front as a function of time, then

$$C_I(d(t),t)=\frac{\partial C_I(d(t),t)}{\partial x}=\frac{\partial^2 C_I(d(t),t)}{\partial x^2}=0 \tag{5}$$

If $I_s(t)$ denotes the cumulative solute entering the soil column across the inlet boundary, then

$$I_s(t)=\int_0^{d(t)} C_I(x,t)\,dx \tag{6}$$

Now integrating equation (1) from 0 to d(t), the left hand side (LHS) is

$$R\int_0^{d(t)} \frac{\partial C_I}{\partial t}\,dx=R\frac{dI_s(t)}{dt} \tag{7}$$

Equation (7) is obtained by using the boundary layer condition, equation (5).

In a similar way, the right hand side (RHS) of equation (1) becomes

$$\int_0^{d(t)} \left(D\frac{\partial^2 C_I}{\partial x^2}-v\frac{\partial C_I}{\partial x}\right)dx=vC_0 \tag{8}$$

Hence equation (1), initial condition, and boundary conditions (inlet boundary and boundary layer) imply that

$$R\frac{dI_s(t)}{dt}=vC_0 \tag{9}$$

or

$$I_s(t)=\frac{vC_0}{R}t \tag{10}$$

One can assume a parabolic or a cubic polynomial concentration profile for a boundary layer solution to the problem. For the cubic polynomial concentration profile, resident concentration is written as

$$C_r(x,t)=a_0(t)+a_1(t)x+a_2(t)x^2+a_3(t)x^3 \tag{11}$$

By using boundary layer conditions, equation (5), the four time coefficients in equation (11) are reduced to a single coefficient, i.e.:

$$C_r(x,t)=a_0(t)\,(1-\frac{x}{d(t)})^3 \tag{12}$$

Equation (12) is valid for $0< x< d(t)$. When $x > d(t)$, $C_r(x, t)=0$. Now $a_0(t)$ can be found by using the inlet boundary condition, equation (3), then

$$a_0(t) = \frac{vd(t)\,C_0}{vd(t)+3D} \qquad (13)$$

Therefore a boundary layer solution to the problem is

$$C_r(x,t) = \frac{vd(t)\,C_0}{vd(t)+3D}\left(1-\frac{x}{d(t)}\right)^3 \qquad (14)$$

Combining equation (14) with equation (6) and integrating yields

$$I_s(t) = \frac{vd(t)^2 C_0}{4\,(vd(t)+3D)} \qquad (15)$$

Combining equation (15) with equation (10) obtains

$$d(t) = \frac{2vt}{R} + \sqrt{\left(\frac{2vt}{R}\right)^2 + \frac{12Dt}{R}} \qquad (16)$$

Equation (16) is obtained by finding the positive root of a parabolic polynomial equation with unknown d(t). Physically d(t) cannot be negative.

Equation (14) and equation (16) complete the boundary layer solution to the problem for the case of cubic polynomial concentration profile. The boundary layer solution is obtained similarly for a parabolic polynomial concentration profile. The corresponding C_r and d(t) are

$$C_r(x,t) = \frac{vd(t)\,C_0}{vd(t)+2D}\left(1-\frac{x}{d(t)}\right)^2 \tag{17}$$

$$d(t) = \frac{3vt}{2R}+\sqrt{\left(\frac{3vt}{2R}\right)^2+\frac{6Dt}{R}} \tag{18}$$

Both equation (16) and equation (18) contain three parameters, v, R, and D. Usually v can be determined accurately from a solute displacement experiment. R and D can be estimated if the change of the boundary layer with time is observed. The boundary layer in this case is physically the depth from the soil surface to solute front. It is experimentally possible to observe the solute front if a dye tracer solution is used. Brilliant blue has proven to be a safe and useful dye for making such a solution (Flury and Fluhler, 1994a and 1994b). It is of interest to compare the boundary layer solution to the CDE with the corresponding exact solution.

The exact solution to the problem (Lindstrom et al., 1967) is

$$\frac{C_r(x,t)}{C_0} = \frac{1}{2}erfc\left[\frac{Rx-vt}{2(DRt)^{0.5}}\right]+\left(\frac{v^2t}{\pi DR}\right)^{\frac{1}{2}}\exp\left[\frac{-(Rx-vt)^2}{4DRt}\right]-f \tag{19}$$

$$f(x,t) = \frac{1}{2}\left(1+\frac{vx}{D}+\frac{v^2t}{DR}\right)\exp\left(\frac{vx}{D}\right)erfc\left[\frac{Rx+vt}{2(DRt)^{0.5}}\right] \tag{20}$$

Comparing the exact solution with the boundary layer solution, it is obvious that the boundary layer solution to the problem is mathematically much simpler than the exact solution. The boundary layer solution is an approximate because it is based on an integral method. In the following section of this paper, the boundary layer solution is compared to the exact solution for a range of values of solute transport parameters, D, R, and v.

Discussion

1. The Change of Boundary Layer with Time

Since equation (16) and equation (18) have similar relationship between boundary layer depth and time discussion here is focused on equation (16). The conclusions of discussion on equation (16) holds true to equation (18). First a simple case of R=1 is considered. This implies that the solutes are nonreactive. Then equation (16) is reduced to

$$d(t) = 2vt + \sqrt{(2vt)^2 + 12Dt} \qquad \textbf{(102)}$$

From equation (21), we can see that the depth of boundary layer for nonreactive solute transport is described by dispersion (D) and convection (v). The sensitivities of d(t) to D and v are shown in Figure 2 (at a given v) and Figure 3 (at a given D). The ratio of D/v is dispersivity. Typical values of dispersivity are 0.5-2 cm in packed laboratory columns and 5-20 cm in the field and they can be considerably larger in regional groundwater transport (Jury et al., 1991; Fried, 1975). In Figure 1, v=0.003 cm/min, dispersivity ranges from 0.5 to 40 cm. At a given average pore-water velocity, the depth of boundary layer (penetration depth of solute) increases with increase of dispersivity. This is expected because increase of dispersion in this case will enhance the advance of the solute front. The point here is that the increase of the depth from 10 to 40 cm of dispersivity is greater than that from 0.5 to 10 cm of dispersivity most of the time. In Figure 3, D=0.03 cm^2/min, the range of dispersivity is the same as in Figure 2. When dispersivity increases from 0.5 to 10 cm there is little increase of the depth. However when dispersivity changes from 10 to 40 cm the increase of the depth is much greater than that in the range of 0.5 to 10 cm. This implies that convection has an important effect on solute transport after v reaches some greater values. Combination of Figure 2 and Figure 3 shows that dispersion has more uniformly effect on solute transport than that of convection.

2. Comparisons of Boundary Layer Solution to Exact Solution

In this section C_0 is assumed to be one. The first case again is the nonreactive solute transport (R=1). At a given pore-water velocity (v=0.001 cm/min), comparisons of the boundary layer solutions to the corresponding exact solutions for dispersivity ranging from 1 to 40 cm are shown in Figure 3-6. The global error in solute concentration is described as the absolute value of difference between exact solution and boundary layer solution. For dispersivity equal to 1 cm, both boundary layer solutions (cubic polynomial and parabolic polynomial concentration profiles) are in good agreement with exact solution (Figure 4). The maximum error of cubic polynomial solution (ME3 for short) is 0.025 and that of parabolic polynomial solution (ME2 for short) is 0.012. Figure 5 shows the comparison for dispersivity of 10 cm. It is obvious that the cubic polynomial solution almost overlaps the exact solution with ME3 of 0.0010. However ME2 is still small at 0.0024. From Figure 6 one can see that for dispersivity of 40 cm the cubic polynomial solution again almost overlaps the exact solution with a ME3 of 0.0015 and while ME2 is 0.0070. From the comparisons one can conclude that the boundary layer solutions (both cubic and polynomial) are in good agreement with exact solutions and that cubic polynomial solutions predict concentration profile better than parabolic polynomial solution. The second case for comparison is reactive solute transport. At a given dispersivity (10 cm), two values of retardation factor, 0.5 and 2, are used. For these values of R both boundary layer solutions predict solute concentration well (Figure 7 and Figure 8). The cubic polynomial solutions for both values of R better match the exact solutions than do the parabolic solutions. ME3 is 0.0034 for R=0.5 and 0.0019 for R=2.0. ME2 is 0.011 for R=0.5 and 0.0065 for R=2.0.

The last case for comparison is nonreactive solute transport again (Figure 9). In this case R=1 and dispersivity is fixed (10 cm). Pore-water velocity is increased by one order of magnitude (from 0.001 to 0.01 cm/min). In this case, the parabolic polynomial solution is better in concentration prediction than that of cubic polynomial solution. The cubic polynomial in this case underestimates the concentration profile and the ME3 is 0.025. However concentration prediction by the parabolic polynomial solution almost overlaps the exact solution with ME2 of 0.0058.

3. Transport Parameter Estimation

The comparisons above indicate that the boundary layer solution can predict concentration profiles well. Because the boundary layer solutions are much simpler mathematically than the corresponding exact solution they may prove to be useful practically in describing solute transport in soil. One application of the boundary layer solution is to estimate solute transport parameters. For this purpose equations (16) or (18) can be used to fit to observation of the advance of solute front with time. Usually pore-water velocity (v) is easy to determine from infiltration data. Thus, the fitting of the solute advance with time can be used to estimate dispersion coefficient and retardation factor. Mathematically, using the boundary layer solution to fit data is much easier than using the exact solution to fit data. Physically, in many cases measuring the advance of solute front is simpler, less time consuming and requires much less technical equipment than does measuring a complete breakthrough curve or resident concentration profile. The advance of solute front with time can be observed visually both in laboratory and field if the tracer solution has a dye. The new method does not require concentration data that is usually either time-consuming (resident and flux concentration in laboratory) or difficult to measure (resident concentration in field conditions). An evaluation of the new method proposed in this paper both under laboratory and field conditions will be performed in the near future.

Conclusions

This study shows that solute transport in a semi-infinite soil column or field profile for flux-type inlet boundary condition can be approximated by boundary layer theory. The boundary layer solution is simpler than the corresponding exact solution. This simplicity is not accidental but results from very close approximation of the specific integral method--boundary layer theory. Generally, the cubic polynomial solution is better in concentration prediction than the parabolic polynomial solution. Both are very similar to the exact solution. An important application of the boundary layer solution is to estimate transport parameters of solute movement through soils both under laboratory and field conditions. This leads to a new method for estimating parameters of solute transport in soils. The observed advance of the solute front with time can be analyzed to determine R and D. The new method provides simplicity, saves time, and overcomes some difficulties in applying the CDE under field conditions.

References

Bresler, E., and A. Naor. 1987. Estimating transport parameters in soils by a maximum likehood approach. Soil Sci. Soc. Am. J. 51: 870-875.

Buchter, B., C. Hinz, M. Flury, and H. Fluhler. 1995. Heterogeneous flow and solute transport in an unsaturated stony soil monolith. Soil Sci. Soc. Am. J. 59: 14-21.

Elprince, A.M., and P.R. Day. 1977. Fitting solute breakthrough equations to data using two adjustable parameters. Soil Sci. Soc. Am. J. 41: 39-41.

Flury, M., and H. Fluhler. 1994a. Brilliant blue FCF as a dye tracer for solute transport studies- A toxicological overview. J. Environ. Qual. 23: 1108-1112.

Flury, M., and H. Fluhler. 1994b. Susceptibility of soils to preferential flow of water: A field study. Water Resour. Res. 30: 1945-1954.

Fried, J.J. 1975 Groundwater Pollution. Elsevier. New York.

Gupta, L.N. 1974. An approximate solution of the generalized stefan's problem in a porous medium. Int. J. Heat Mass Transfer. 17: 313-321.

Kumar, I.J., and H.N. Narang. 1967. A boundary-layer method in porous body heat and mass transfer. Int. J. Heat Mass Transfer. 10: 1095-1107.

Jury, W.A., and G. Sposito. 1985. Field calibration and validation of solute transport models for the unsaturated zone. Soil Sc. Sac. Am. J. 49: 1331-1341.

Jury, W.A., W.R. Gardner, and W.H. Garder. 1991. Soil Physics. John Wiley & Sons, Inc. New York.

Kool, J.B., J.C. Parker, and M.Th. van Genuchten. 1987. Parameter estimation for unsaturated flow and transport models--a review. J. Hydrol. 91: 255-293.

Lindstrom, F.T., R. Haque, V.H. Freed, and L. Boersma. 1967. Theory on the movement of some herbicides in soil: Linear diffusion and convection of chemicals in soils. Environ. Sc. Technol. 1:561-565.

Parker, J.C., and M.Th. van Genuchten. 1984. Determining transport parameters from laboratory and field tracer experiments. Virginia Agric. Exp. Stn. Bull. 84-3.

Rifai, M.N.E., W.J. Kaufman, and D.K. Todd. 1956. Dispersion phenomena in laminar flow through porous media. Inst. of Eng. Res. Ser. no. 93(2). Sanitary Eng. Res. Lab. Univ. of Calif., Berkeley.

Schnable, R.R., and E.B. Richie. 1987. Elimination of time assignment bias in estimates of dispersion coefficient. Soil Sci. Soc. Am. J. 51: 302-304.

van Genuchten, M. Th., and J.C. Parker. 1984. Boundary conditions for displacement experiments through short laboratory soil columns. Soil Sci. Soc. Am. J. 48: 703-708.

van Genuchten, M. Th., and J.C. Parker. 1994. Reply to "Comments on 'Boundary conditions for displacement experiments through short laboratory soil columns'". Soil Sci. Soc. Am. J. 58: 991-993.

Yamaguchi, T., P. Moldrup, and S. Yokosi. 1989. Using breakthrough curves for parameter estimation in the convection-dispersion model of solute transport. Soil Sc. Soc. Am. J. 53: 1635-1640.

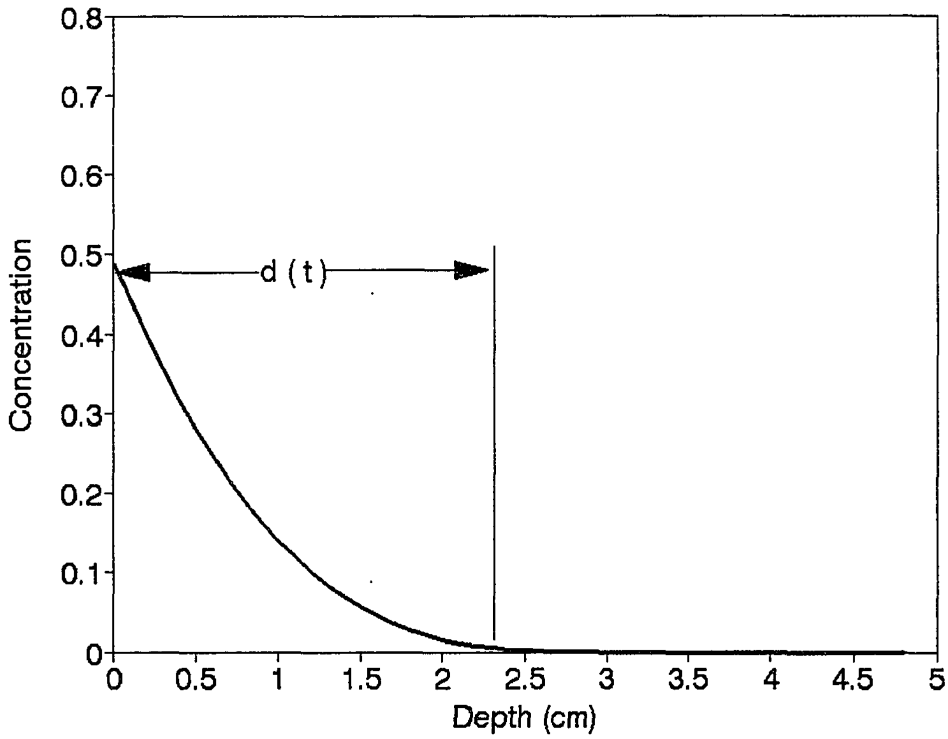

Figure 1. A schematic diagram of solute boundary layer.

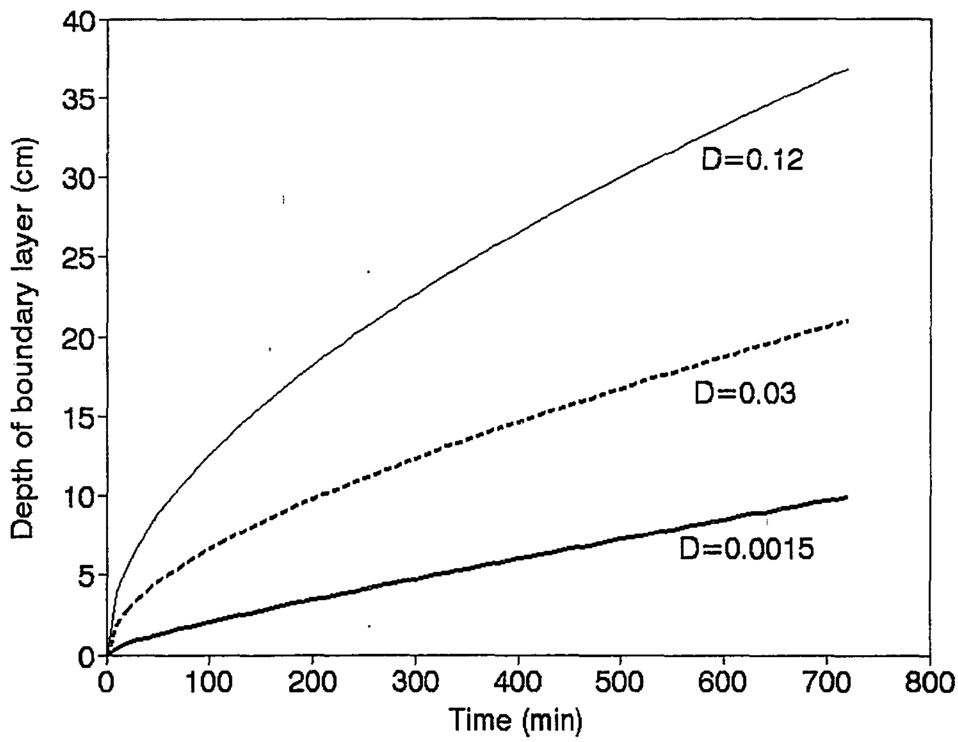

Figure 2. Effect of dispersion coefficient on the relation of boundary layer with time (v=0.03 cm/min)

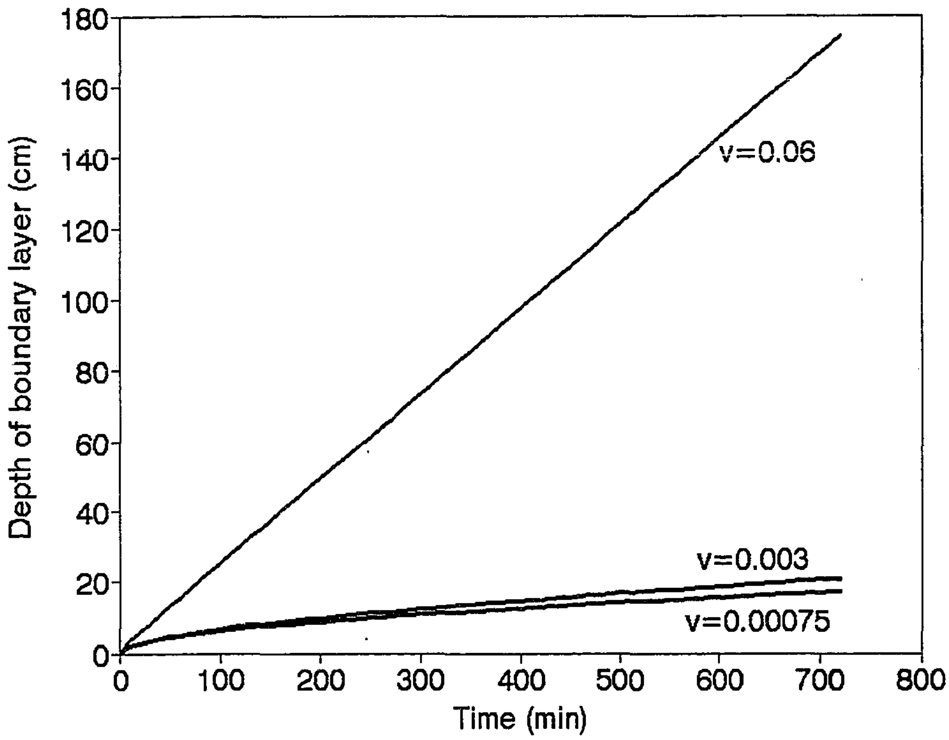

Figure 3. Effect of pore water velocity on the relation of boundary layer with time (D=0.03 cm^2/min).

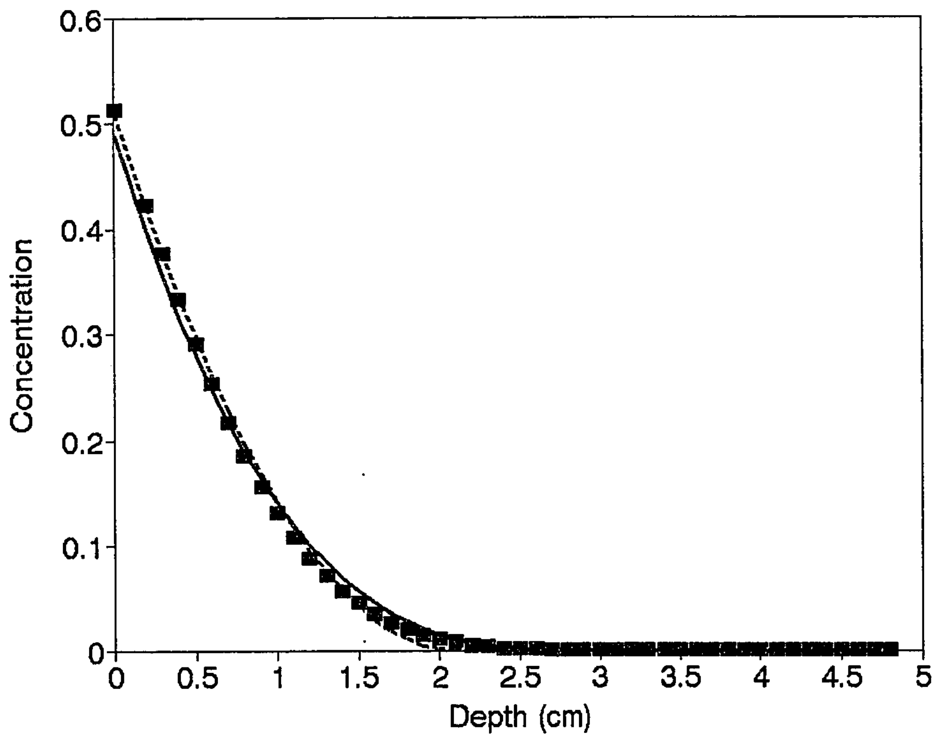

Figure 4. The comparison of concentration profiles for nonreactive solute transport with dispersivity of 1 cm, filled square--exact solution, solid cure--cubic boundary layer solution, dashed curve--parabolic boundary layer solution (t=300 min).

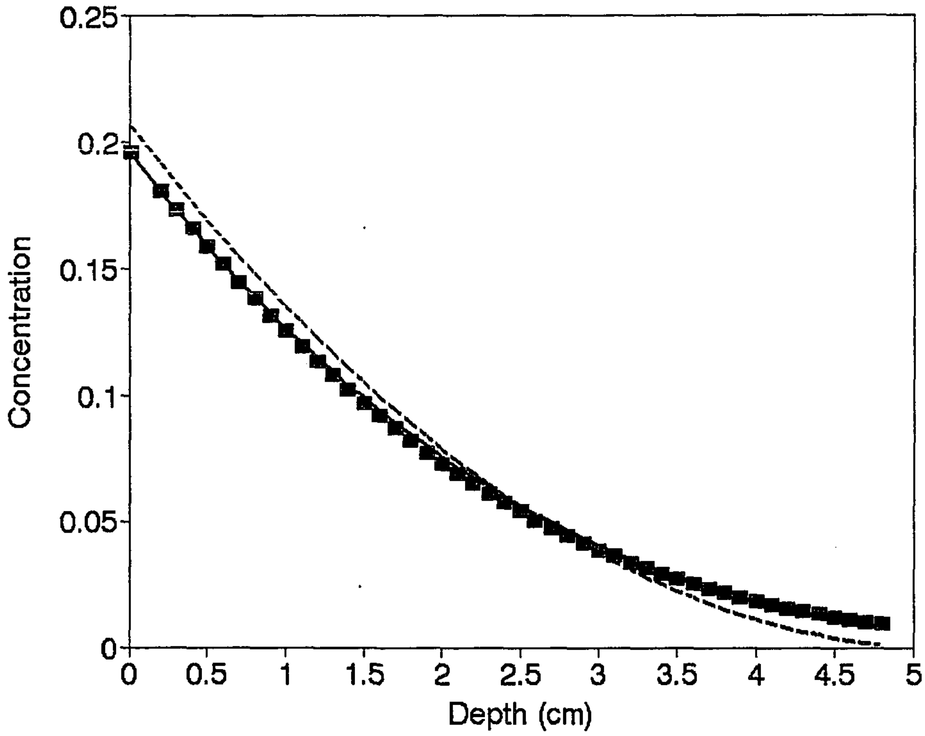

Figure 5. The comparison of concentration profiles for nonreactive solute transport with dispersivity of 10 cm, filled square--exact solution, solid cure--cubic boundary layer solution, dashed curve--parabolic boundary layer solution (t=300 min).

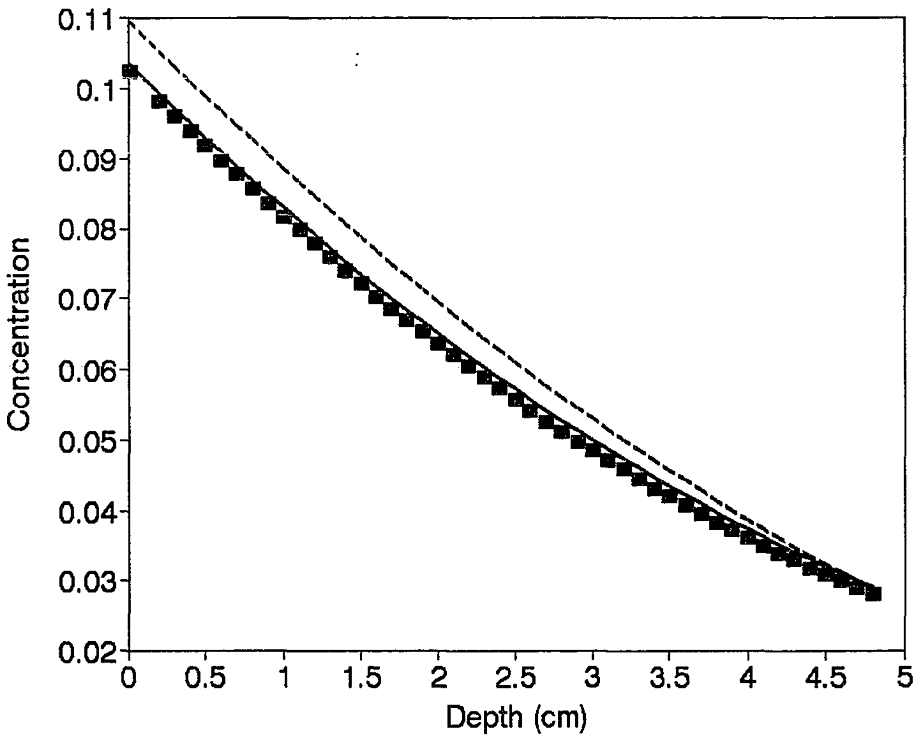

Figure 6. The comparison of concentration profiles for nonreactive solute transport with dispersivity of 40 cm, filled square--exact solution, solid cure--cubic boundary layer solution, dashed curve--parabolic boundary layer solution (t=300 min).

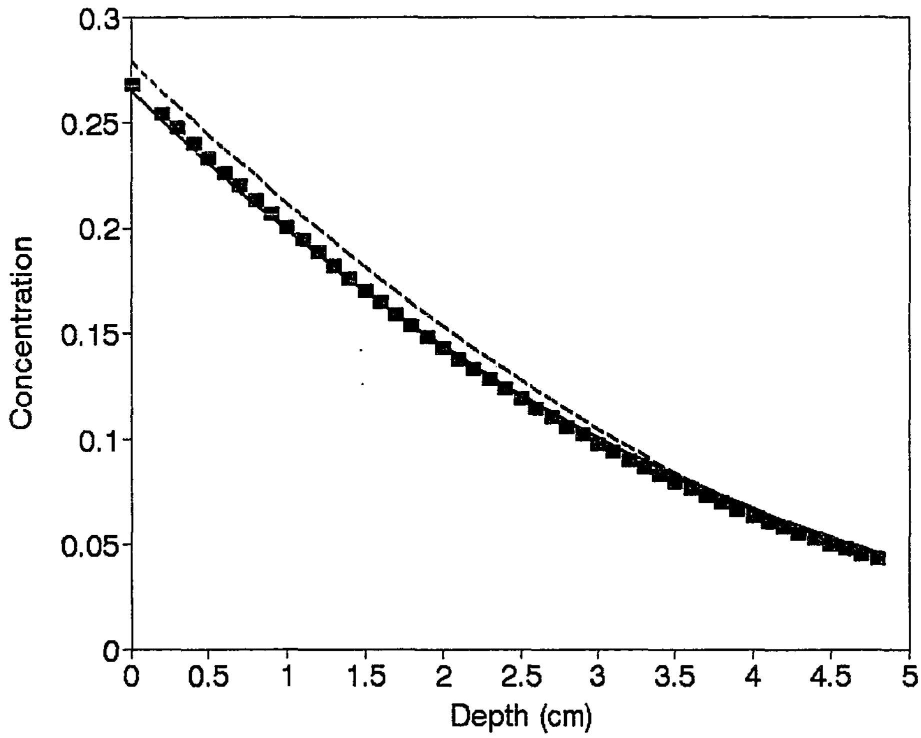

Figure 7. The comparison of concentration profiles for reactive solute transport (R=0.5) with dispersivity of 10 cm, filled square--exact solution, solid cure--cubic boundary layer solution, dashed curve--parabolic boundary layer solution (t=300 min).

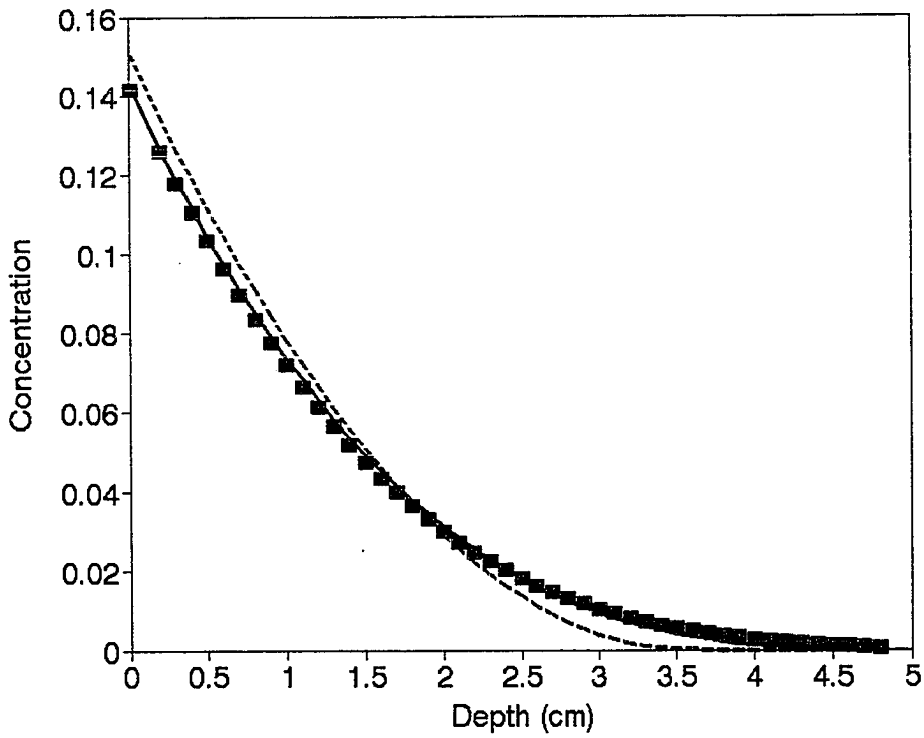

Figure 8. The comparison of concentration profiles for reactive solute transport (R=2.0) with dispersivity of 10 cm, filled square--exact solution, solid cure--cubic boundary layer solution, dashed curve--parabolic boundary layer solution (t=300 min).

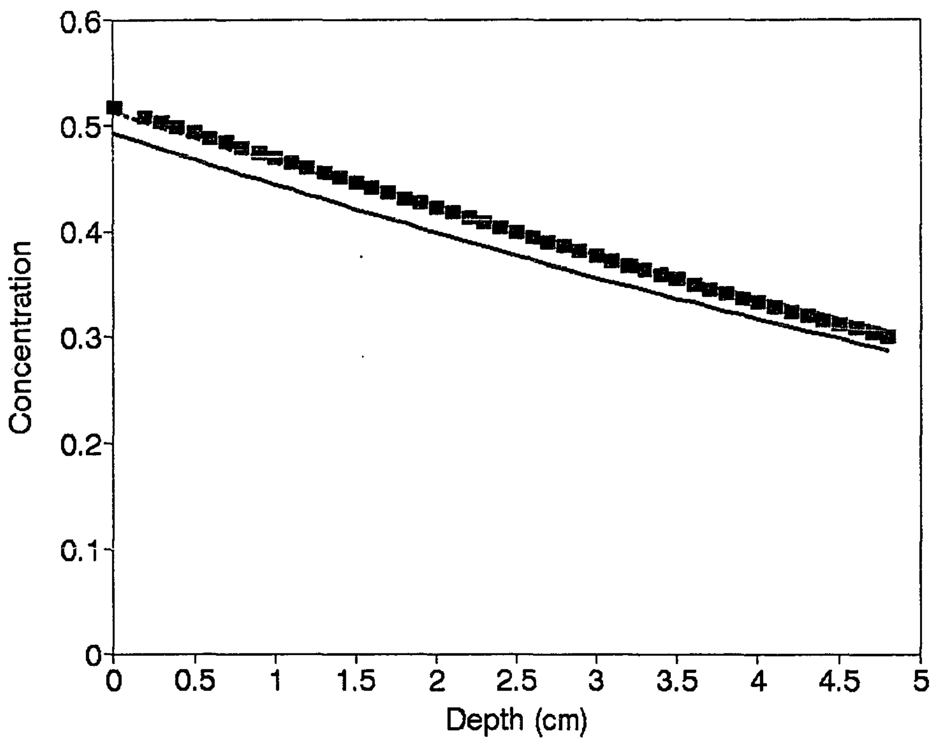

Figure 9. The comparison of concentration profiles for nonreactive solute transport with dispersivity of 10 cm and pore water velocity of 0.01 cm/min, filled square--exact solution, solid cure--cubic boundary layer solution, dashed curve--parabolic boundary layer solution (t=300 min).

CHAPTER 8. GENERAL CONCLUSIONS

Transport processes of heat, water, and chemicals in soils are involved in this study in such a way to find simple and new analytical or approximate solutions to the corresponding transport problems. Analytical solutions are further manipulated to estimate the corresponding transport properties.

An analytical solution to coupled conduction and convection heat transfer problem is obtained by using Fourier transformation. Results from the analytical solution compare well to observations from a field infiltration experiment with natural temperature variations.

A general similarity solution is provided in this research for horizontal infiltration-redistribution processes. The solution is closed form and flexible. The general similarity solution is tested by comparing to a numerical solution. A new and simple method to determine soil water diffusivity is developed based on the simplicity of the general similarity solution. The new method only requires measuring advance of wetting front with time. The general similarity diffusivities of five soils compare well to those determined by Boltzmann transformation. The new method does not require soil water diffusivity to be zero at the initial water content. This represents an improvement over the earlier methods that give a zero diffusivity at initial water content no matter how high the initial water content.

An infiltration method for estimating soil hydraulic properties is also presented in this study. The new method is developed by solving Richards equation for horizontal infiltration of water in soils that are described by van Genuchten Model. The estimated hydraulic properties for six soils ranging from sandy loam to clay loam (water characteristic curve and unsaturated hydraulic conductivity) by the infiltration method are in good agreement with the observed data of hydraulic properties. The infiltration method provides a simple, accurate, and fast procedure for the estimating soil hydraulic properties.

An approximate solution to the classical convection-dispersion equation is obtained by boundary layer theory. The boundary layer solution compares well to the exact solution. A procedure for estimating dispersion coefficient and retardation factor is developed based on the simplicity and flexibility of the boundary layer solution. The new method may prove to be useful because it is applicable both to soil columns and field soils.

All of the solutions developed in this dissertation have application to heat, water or chemical transport in natural or laboratory conditions. The solutions are developed such that when applied to soil studies useful transport properties can be determined. The new methods described here represent improvement over previous methods. The new methods are easy to use and the time required is shorter than the existing methods.

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